US High Production Volume Chemical Program

Summary
For
Polyethylbenzene Bottoms

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For

American Chemistry Council
Ethylbenzene Panel

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TABLE OF CONTENTS

Tables

Ethylbenzene Panel

Producers of Polyethylbenzene Bottoms

Chevron Phillips Chemical Company LP

The Dow Chemical Company

INEOS Styrenics (formerly Innovene and BP Amoco Chemical Company)

Lyondell Chemical Company

NOVA Chemicals Inc.

TOTAL Petrochemicals USA, Inc. (formerly ATOFINA Petrochemicals Inc.)

EXECUTIVE SUMMARY

The Polyethylbenzene Bottoms [PEB Bottoms] stream is a co-product of ethylbenzene manufacture. Ethylbenzene is produced by the alkylation of benzene with ethylene. Side reactions produce di-, tri- and polyethylbenzene as well as butylbenzene and other alkylaromatics. After removal of ethylbenzene, the remaining stream is separated into a diethylbenzene-rich distillate stream and a Bottoms stream described as benzene, ethylenated, residues or Polyethylbenzene Bottoms. The composition of these Bottoms streams varies with the manufacturer and processing. The material is a liquid with low vapor pressure under ambient conditions. Likely routes of exposure are inhalation and accidental dermal contact. Workplace exposure is limited because of the low vapor pressure of the stream and because production occurs primarily in a closed system. The general population is unlikely to be exposed to PEB Bottoms because there are no direct consumer uses for this material. PEB Bottoms is subject to USEPA and state regulations that limit volatile organic compound emissions and the heavy liquid control requirements of the fugitive emissions standard.

The PEB Bottoms sample used in this HPV testing program was a blend of equal volumes of 6 PEB Bottoms samples from 6 different suppliers. Physical chemical properties, biodegradation and aquatic toxicity studies were performed using the PEB Bottoms blended sample or modelled using data on constituent hydrocarbons. These hydrocarbons have a very low potential to hydrolyze and do not degrade directly. The calculated half-lives of component hydrocarbons suggest the PEB Bottoms atmospheric half-life would be approximately 1 day, as a result of indirect hydrolysis by hydroxy radical attack. Fugacity modelling demonstrated that constituent hydrocarbons in PEB Bottoms partition either into air or soil at percentages depending in large part on the number of ring constituents in the molecule with only a small percentage of any compound partitioning into water or sediment. PEB Bottoms is not readily biodegradable. Exposure of aquatic species to water accommodated fractions (WAF) of PEB Bottoms indicates that PEB Bottoms is toxic to very toxic to aquatic life and that *Daphnia* and algae may be somewhat more sensitive to PEB Bottoms WAF exposure than freshwater fish. Using the acute toxicity hazard to *Daphnia* to estimate a chronic toxicity value, PEB Bottoms was determined to pose a chronic toxicity hazard to invertebrates as well. However PEB Bottoms is not generally used in emissive applications, and thus would not be expected to enter the environment.

In acute mammalian studies, a sponsor's PEB Bottoms sample was minimally toxic by the oral and dermal routes of exposure although some skin irritation was seen. PEB Bottoms induced gene mutation in bacteria but did not induce chromosome aberrations in mammalian cells in culture. Effects in the OECD 422 Combined 28 day Repeated Dose Toxicity Study with Reproductive/Developmental Screening by the oral route included decreased adult body weight and body weight gain, decreased food consumption, increased kidney (males only), liver and thyroid weights, and decreased thymus weights which correlated with microscopic changes. Neurobehavioral parameters were not affected by PEB Bottoms treatment. Male and female fertility was comparable to control values although mean gestation duration was increased in high dose females. Adverse trends in some reproductive parameters (i.e. implantation sites, number of pups born, live litter size) suggested the possibility of PEB Bottoms-induced reproductive effects but no neonatal toxicity affecting offspring survival, physical condition or body weights occurred.

This body of data fulfils the Tier 1 testing recommendations of the HPV program. In consideration of the controlled production and usage, and limited exposure potential of PEB Bottoms, the screening level information provided in this report is adequate to characterize the potential hazard of this substance.

1 SUBSTANCE DESCRIPTION AND HAZARD CHARACTERIZATION APPROACH

1.1 Substance Identification

Polyethylbenzene Bottoms stream [PEB Bottoms] is a complex aromatic hydrocarbon stream that is a co-product of ethylbenzene manufacture. Ethylbenzene is produced through alkylation of benzene with ethylene. In addition to the production of ethylbenzene, there are side reactions that involve the reaction of ethylene with ethylbenzene to produce diethylbenzene and further alkylations to produce triethylbenzene and polyethylbenzene. In addition, butylbenzene and other alkylaromatics may be formed in varying amounts. After the ethylbenzene is removed, the remaining stream is separated into a diethylbenzene-rich stream and a Bottoms stream. This co-product Bottoms stream is described as Benzene, ethylenated, residues (CAS# 68987-42-8), also called Polyethylbenzene Bottoms or Polyethylbenzene Residue. This material is a Class II complex mixture. PEB Bottoms is included in a group of substances identified under the TSCA code as "UVCB", "substances of unknown or variable composition, a complex reaction product, or a biological material".

Table 1. CAS Number and CAS Names Associated with PEB Bottoms

CHEMICAL NAME	OTHER NAMES	CAS #
Benzene, ethylenated, residues	Polyethylbenzene Bottoms Polyethylbenzene Residue PEB BOTTOMS Bottoms PEB BOTTOMS Residue	68987-42-8

The composition of PEB Bottoms is expected to consist of variable amounts of primarily the components listed below in Table 2. The list of components and content ranges is based on a composite of capillary GC analyses of samples submitted by six participating companies to BP Amoco Analytical Technology (BP Amoco, 2000).

Table 2. Composition of PEB Bottoms Samples

Composition	Wt%
Diphenylethanes	15 – 32
Diphenylmethanes	<0.5 – 31
Other diphenylalkanes	7 –17
Ethyl diphenylethanes & diethylbiphenyls	9 –21
Polyethylbenzenes	<0.1 – 19
Triethylbenzenes	<1 – 26
Diethylbenzenes (m-, o-, p-)	<0.1 –4
Butylbenzenes	<0.1
Other alkylbenzenes	9 – 24
PNAs (3-ring)	0.4 – 11
Ethylbenzene	<0.1
Benzene	<0.1
Paraffins/Naphthenes	<0.3
Total of unidentified components each present at <0.1%	3 – 5

Please note that the Diethylbenzene Rich-Streams (CAS Registry #25340-17-4 and 68608-82-2) are addressed separately under the HPV Chemical Program.

The PEB Bottoms sample used in this HPV testing program was a blend of equal volumes of six PEB Bottoms samples from 6 different suppliers. The blended sample is a clear, yellow liquid under ambient conditions. Pertinent information concerning preparation and characterization of this blended sample is available in Appendix 1.

Table 3. Characterization of PEB Bottoms Blended Sample

Component	Wt %
diethylbenzene	0.01
1,3,5-triethylbenzene	6.20
1,2,4-triethylbenzene	7.23
cyclohexylbenzene	0.66
diphenylmethane	20.45
1,1'-diphenylethane	25.42
1,2-diphenylethane (bibenzyl)	7.98
1,1'-diphenylpropane	2.42

From gas chromatography/mass spectrometry (GC/MS) analysis of the blended sample, 8 specific components were identified, comprising approximately 70% of the PEB Bottoms blended sample. Additional component characterization was not possible due to the complexity of the material, containing additional peaks with very similar retention times and weight % values less than 1%.

1.2 Purity/Impurities/Additives

PEB Bottoms is an extremely complex mixture of hydrocarbons in the C5 – C14 carbon range; hence a purity description of this substance is not applicable. Typically there are no unique impurities or additives present in this stream.

1.3 Physico-Chemical properties

The physico-chemical properties for PEB Bottoms have been measured. Robust summaries for Physico-Chemical properties studies are provided in Appendix 2, pp. 29-37.

Table 4. Summary of Measured Physico-Chemical Properties of PEB Bottoms

Endpoint	Method	Result
Freezing Point	OECD 102	-58.8 ± 0.0^0C
Boiling Point [see table 4a]	OECD 103	262.2 ± 0.3^0C
Vapor Pressure	OECD 104	$< 10^2$Pa (< 0.7mm Hg) at 10, 20, or 30^0C
Log P_{ow}	OECD 117 [HPLC method]	4.08 to 6.01 @ 20^0C
Water Solubility	OECD 105	29.5 ± 1.4mg/L @ 20 ± 0.5^0C

Table 4a. Modeled Boiling Point Values for Selected Chemicals Contained in PEB Bottoms

	Boiling Point, ^{0}C	
Chemical Name	**Measured**	**Modeled**
Diethylbenzene	181.0	191
Cyclohexylbenzene	240.1	238
1,2,5-triethylbenzene	215.9	230
1,2,4-triethylbenzene	218.0	230
Diphenylmethane	265.0	269
1,1-diphenylethane	272.6	276
1,2-diphenylethane	284.0	285
1,1-diphenylpropane	281.6	291

Values determined by EPIWIN computer model; V3.12, subroutine MPBPWIN, V 1.41 (US EPA, 2000) Measured values were cited in the EPIWIN experimental database.

1.3.1 Freezing Point [Robust Summary, Appendix 2 p. 30]

The freezing point was determined in triplicate following ASTM method D 1015-99 (OECD method 102; 1995). As the test substance cooled, the temperature was recorded every 15 seconds. A temperature versus time plot was prepared for each replicate determination and freezing point was determined from the equilibrium portion of the freezing curve. The freezing point of PEB Bottoms was determined to be –58.8± 0.0^{0}C.

1.3.2 Boiling Point

Measured [Robust Summary, Appendix 2 p. 31]

Boiling point was measured in a Mettler FP900 Thermosystem consisting of a Mettler FP81HT MBC Cell attached to a Mettler FP90 Central Processor (OECD method 10; 1995). PEB BOTTOMS was added to a boiling point tube to a height of 15-18mm. A boiling capillary was inserted into the boiling point tube and the tube was analyzed by inserting the tube into the center slot of the instrument. The sample was analyzed starting at 258^{0}C and increasing in +0.2^{0}C/minute until the boiling point was reached. The boiling point recorded was calculated by the instrument using the actual boiling temperatures and barometric pressure (99.2 kPa) measurements, and corrected to standard pressure (101.325 kPa) automatically by the instrument. By this method the boiling point of PEB Bottoms was determined to be 262.2±0.3^{0}C.

Modeled Range [Robust Summary, Appendix 2 p. 33]

Because PEB Bottoms is a blended sample comprised of numerous hydrocarbon components, a boiling point range was also determined. The calculated boiling points [by EPIWIN V3.12, subroutine MPBPWIN, version 1.41] for some representative constituents that are present in PEB Bottoms range from 191 to 291°C [Table 4a.]. The measured boiling points of these same constituents range from 181 to 284°C. These data offer an indication of a range that encompasses the boiling points of PEB BOTTOMS.

1.3.3 Vapor Pressure [Robust Summary, Appendix 2 p. 34]

Vapor pressure of PEB Bottoms was determined using a Terranova model 908A dual capacitance diaphragm gauge controller, Baratron pressure transducer, Franklin electric vacuum pump model 4401007400, and 100-mL long-necked, round bottom flasks with sidearm in accordance with OECD method 104 (1995). At the initiation of the study, approximately 25ml PEB Bottoms were added to the test flask. The sample was degassed at reduced temperature and the flask valve was opened for several minutes to remove any liberated air then was closed. Following 30 minutes of

immersion in the water bath set at 10°C, the vapor pressure reading was recorded then recorded again at temperatures of the waterbath adjusted to 20 and 30°C. This procedure was repeated for a second replicate determination. The vapor pressure of PEB Bottoms Blend was determined to be less than 90 Pa at 10, 20, and 30°C, respectively. All pressure readings at 10, 20, and 30°C were less than 0.7mm Hg. The vapor pressure of PEB Bottoms was less than 10^2 Pa at each of the temperatures evaluated.

1.3.4 Partition Coefficient: Log P_{ow} [Robust Summary, Appendix 2 p. 36]

The partition coefficient of PEB Bottoms was determined using OECD 117, HPLC method (2004). Fifty microliter samples of an 11.5µg/mL solution of PEB Bottoms in mobile phase were injected into the HPLC, and the emergence of the material was observed using UV detection (λ = 210 nm). Eight reference compounds were used to generate the linear relationship between log k (k = capacity factor) and log Pow. Using the HPLC retention time for the peak of the test substance, the log k was determined, and the log Pow value was calculated using a linear equation developed from the reference compounds. HPLC analysis of the test substance resulted in multiple peaks, thirteen of which were attributed to PEB Bottoms. The log P_{ow} values for each of the peaks of the test substance were determined by substituting their experimentally determined log k values into the equation derived from the log k versus log P_{ow} graph constructed from the reference standards. The Log P_{ow} range was 4.08 to 6.01 at 20^0C.

1.3.5 Water Solubility [Robust Summary, Appendix 2 p. 37]

Water solubility was measured using the shake flask method described in OECD method 105 (1995). Test samples were prepared by combining 3 mL of PEB Bottoms and 33 mL of reagent water in each of three, 40-mL plastic centrifuge tubes. The samples were capped and placed on an orbital shaker water bath set at 30 °C and agitated. One replicate was removed from the shaker after approximately 24, 48, and 72 hours and placed on a shaker at 20 °C. Five days after placing the first sample on the shaker at 20°C, the three samples were removed, centrifuged and the aqueous layers were removed to scintillation vials. Twenty mL of each sample was extracted and analyzed by gas chromatography. Analyses were done using gas chromatography with a flame ionization detector. Responses of standards and samples were calculated as the sum of the responses from six marker peaks within the PEB Bottoms chromatogram. The solubility measurements at 48 and 96 hours averaged 30.7 mg/L and 28.4 mg/L, respectively. The final water solubility value was the overall mean of the 48 and 96-hour sample determinations. Water solubility was 29.5 ± 1.4 mg/L at 20 ± 0.5°C.

1.4 Hazard Characterization Approach

The Panel conducted a search of the published literature and found no test data on this material. Panel members searched company files for unpublished data and found data on endpoints that are not part of the HPV dataset (e.g. irritation) or data that are not sufficiently robust to meet the standards of the HPV program. The Panel also considered whether this material could be combined in a category with other HPV chemicals for purposes of the HPV program, but since this material is unique to the ethylbenzene manufacturing process and does not have a composition common with other HPV materials, it was not feasible to combine this material into a category combining multiple CAS numbers for hazard assessment or HPV testing.

Since no individual component is present at greater than 20% in PEB Bottoms, prediction of health or environmental toxicity based on a component or components was not considered appropriate or adequate for the hazard characterization. The objective of the Panel's participation in the HPV program was to identify and develop sufficient test data and/or other information to adequately

characterize the human and environmental fate for PEB Bottoms in accordance with the EPA HPV Program.

2 GENERAL INFORMATION ON EXPOSURE

2.1 Production Volumes and Use Pattern

Sponsors of the American Chemistry Council Ethylbenzene Panel's HPV program produce PEB Bottoms. This stream is a complex aromatic hydrocarbon concentrate with variable composition. The components of the stream are largely substituted alkyl benzenes and substituted diphenylalkanes.

Table 5. PEB Bottoms Nomenclature

Industry Stream Name	CAS Number	CAS Name
Polyethylbenzene Bottoms	68987-42-8	Benzene, ethylenated, residues

Ethylbenzene is produced through alkylation of benzene with ethylene. In addition to the production of ethylbenzene, there are side reactions that involve the reaction of ethylene with ethylbenzene to produce diethylbenzene, and, to a much lesser extent, further alkylations to produce triethylbenzene and polyethylbenzene. In addition, butylbenzene and other alkylaromatics may be formed in varying limited amounts.

In the Ethylbenzene process, benzene is reacted with ethylene in the alkylation reactors section of the process. Unreacted benzene and product ethylbenzene are removed from the alkylation reactor effluent. The remaining stream is separated by distillation into a diethylbenzene-rich distillate stream and a Bottoms stream. This Bottoms stream is the Polyethylbenzene Bottoms (PEB Bottoms) and consists of the higher boiling reaction byproducts of the ethylbenzene production process.

PEB Bottoms production, as reported by the six sponsors[1] who provided data for this assessment, was 60.9 million lbs in 2004. This screening level exposure assessment is based on information received from six sponsors of the stream and upon other available information.

Storage and Transportation: When shipped between industrial sites, PEB BOTTOMS is transported in bulk quantities by rail in tank cars or tank trucks. Typically, the stream is shipped by each of the manufacturers to relative few locations (1 to 3 customer sites).

Use: Primary Uses of PEB BOTTOMS (2004), based on information collected from the manufacturers for this assessment are shown in Table 6. These percentages are expected to be representative of the total stream production.

[1] Production and use data was obtained from 6 producers who are members of the Ethylbenzene Panel's HPV program of the stream.

Table 6. PEB Bottoms Use (2004)

Use	% Of Total
Industrial Heat Transfer Fluid	30%
Chemical Intermediate	22%
Industrial Processing Aid	19%
On Site Fuel Oil	17%
Industrial Seal Fluids	11%
Marine or Industrial Fuel	1%

The producers of the stream reported no consumer uses of PEB Bottoms.

Route of Potential Exposure: PEB Bottoms is a liquid with a low vapor pressure[2] at ambient conditions. Inhalation and accidental dermal contact are possible routes of occupational exposure to PEB Bottoms.

Sources of Potential Exposure: The potential exposure to PEB Bottoms is limited for workers at ethylbenzene plants where the stream is manufactured, in part because of the low vapor pressure of the stream and because the manufacturing process is generally a closed system.

For industrial workers at these facilities, the most likely exposure potential occurs through inhalation of low-level concentrations in air of vapors that escape from the manufacturing process, such as fugitive emissions from valve packing and pump seals or during operations such as sampling and loading bulk transportation vessels (tank cars and tank trucks); or from storage tank emissions.

Exposure potential information at facilities that receive and use the PEB Bottoms stream was not available for this assessment, but is expected to be similar to that at the manufacturing facility.

Controls that Limit Exposure: Potential exposure to PEB Bottoms is limited because of the low vapor pressure of the stream and because the manufacturing process is generally a closed system. The flammability of the stream also provides an incentive to limit emissions.

The Occupational Safety and Health Administration (OSHA) has not established an 8-hour time-weighted (8-hr TWA) personnel exposure limit (PEL) for PEB Bottoms or for the primary hydrocarbon components that make up the mixed stream. Similarly, the American Conference of Governmental Industrial Hygienists has not adopted an 8-hr TWA threshold limit value (TLV) or a short-term exposure limit (STEL) for the stream or the primary components.

One manufacturer of mixed Diethylbenzenes reported use of an industrial hygiene program that assesses worker exposure to diethylbenzene, a minor component of the mixed stream.

Ambient Concentration Data: Hydrocarbon components in the PEB Bottoms streams are slightly soluble in water and therefore groundwater contamination is possible in the event of spills or leaks from processing, transportation or storage equipment or from water effluents at industrial facilities.

[2] The vapor pressure of combined samples of PEB Bottoms from several manufacturers was determined to be less than 90 Pa (less than 0.7 mmHg) at 10, 20 and 30 degrees C.

Ambient air concentrations of the PEB Bottoms near facilities producing and using PEB Bottoms is expected to be relatively low, in part because of the low volatility of the stream. Ambient air monitoring data are not available for this HPV stream since it is a complex hydrocarbon mixture. Ambient air monitoring data are also not generally available for the primary components.

Diphenylmethane is a component of PEB Bottoms, and may be present in the stream at concentrations up to 31%. Information about diphenylmethane is available in the National Library of Medicine's Hazardous Substance Database (HSDB)[3]. The sources of diphenylmethane described in the HSDB include sources other than or in addition to PEB Bottoms. According to the HSDB, diphenylmethane is manufactured by various processes (e.g. from benzene and formaldehyde in the presence of sulfuric acid) and used for example in the production of dyes, perfumes, soap, and as a solvent for cellulose lacquers. Diphenylmethane emitted from PEB Bottoms contributes (at most) to only a small portion of the concentrations indicated in the HSDB. The following is a partial summary of information for diphenylmethane (Benzene, 1,1'-methylenebis-) that was obtained from the HSDB.

- "DRINKING WATER: 1,1'-Methylenebisbenzene has been identified, but not quantified in drinking water. [Kool HJ et al.; 1982] In a survey of 14 treated drinking water supplies of varied sources in England, 1,1'-methylenebisbenzene was detected in one supply which came from a potentially polluted groundwater supply. (Fielding M et al., 1981) Samples of Ottawa tap water taken in January and February 1978 contained 1.4 and 2.8ng/l of 1,1'-methylenebisbenzene. (Benoit F.M et al., 1978)

- EFFLUENT CONCENTRATIONS: In a comprehensive survey of wastewater from 4000 industrial and publicly owned treatment works (POTWs) sponsored by the Effluent guidelines Division of the US EPA, 1,1'-methylenebisbenzene was identified in discharges of the following industrial category (frequency of occurrence, median concentration in ppb): timber products (1; 70.9), paint and ink (3; 34.8), printing and publishing (1; 38.5), coal mining (2; 75.7), organics and plastics (10; 356.6), plastics and synthetics (1; 28.6), rubber processing (1; 207.1), pesticides manufacture (1; 281.4), pharmaceuticals (6; 204.7), explosives (2; 40.6), electronics (1; 43.8), oil and gas extraction (1;43.8), organic chemicals (3; 1183.3), publicly owned treatment works (20; 18.2)(1). The highest effluent concentration was 29,554 ppb in the paint and ink industry. (Shackelford WM et al., 1980)

- FOOD SURVEY VALUES: 1,1'-Methylenebisbenzene has been detected in the volatile component of baked potato (Coleman EC et al., 1981).

- FISH/SEAFOOD CONCENTRATIONS: 1,1'-Methylenebisbenzene was identified, but not quantified, in fish in the Great Lakes (Konasewich D et al., 1978)

- OTHER ENVIRONMENTAL CONCENTRATIONS: 1,1'-Methylenebisbenzene has been found in fly ash from a municipal incinerator in Toronto Canada (Karasek FW et al., 1987).

Estimates of Potentially Exposed Workers: Data not available.

[3] Hazardous Substances Data Bank (HSDB), a database of the National Library of Medicine's TOXNET system (http://toxnet/nlm.nih.gov) downloaded May 13, 2006.

2.2 Environmental Exposure and Fate

2.2.1 Sources of Environmental Exposure

Emissions of PEB Bottoms may occur as a result of fugitive emissions from the process, such as from valve packing and pump seals. Other potential emission may result during operations such as sampling, storage and loading bulk transportation vessels (tank cars and tank trucks); or during infrequent opening of equipment for maintenance. Because of the low vapor pressure of PEB Bottoms, storage and loading operation vents are not typically routed to a recovery or control device and in some cases process vents are not controlled. However, emissions of the PEB Bottoms or components of the stream are expected to be low from these sources. One sponsor indicated that material balances by the technology provider did not show any diethylbenzene or polyethylbenzene substances in the atmospheric process vent from a distillation system vacuum ejector condenser. Hydrocarbon components of the streams (individual hydrocarbon species) may also be found at low concentration levels in water discharges from manufacturing or use facilities.

Flammability of PEB Bottoms provides major incentive to limit emissions from process equipment at industrial facilities.

PEB Bottoms is a volatile organic compound (VOC) and is subject to USEPA and state environmental regulations that limit VOC emissions. The USEPA new source performance standards of 40CFR Part 60 limit emissions of VOC at new or modified process units. Subpart VV of 40CFR Part 60 limits emission from equipment leaks, Subpart NNN limits emissions from distillation operations. Because of the streams low vapor pressure, the heavy liquid control requirements of the fugitive emissions standard applies. Facilities that produce and use PEB Bottoms are also typically subject to state operating permits and regulations that further limit VOC emissions.

Industrial emissions of PEB Bottoms and the primary components in the stream are not reported to the EPA in the Toxics Release Inventory (TRI). This inventory was established under the Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA) and expanded by the Pollution Prevention Act of 1990.

One sponsor of the stream reported 26.8 pounds of PEB Bottoms emissions from their production facility for the year 2004. A second sponsor reported (for 2004) the following emissions of components that may be included in PEB Bottoms. Note that these emissions estimates for both facilities are from the ethylbenzene production facility and not specifically from the PEB Bottoms stream.

Table 7. 2004 Total Ethylbenzene Plant Emissions of Components found in PEB Bottoms Reported by One Producer's Facility

Components of PEB Bottoms	Emissions, lbs/yr
Benzene: (1-Methylethyl)-	0.1
Benzene: 1,1'-(1,2-Ethanediyl)Bis-	0.3
Benzene: 1,1'-Ethylidenebis-	0.3
Benzene: Butyl-	54.5
Benzene: Diethyl-	642.1
Benzene: Methyl	5.0
Benzene: Triethyl	70.4
Polyethylbenzenes	887.5

2.2.2 Photodegradation [Robust Summary, Appendix 2 pp. 39-42]

Direct photodegradation [Robust Summary, Appendix 2 pp. 39]: A prerequisite for direct photodegradation is the ability of one or more bonds within a chemical to absorb ultraviolet (UV)/visible light in the 290 nm to 750 nm range. Light wavelengths longer than 750 nm do not contain sufficient energy to break chemical bonds, while wavelengths below 290 nm are shielded from the earth by the stratospheric ozone layer (Harris, 1982a). The majority of the constituents identified in PEB Bottoms consist of various isomers of alkylbenzene and diphenyl structures. Single ring aromatics do not absorb sufficient light energy above 290 nm to cause photolysis. Therefore, those types of constituents are not subject to photolysis. Similarly, diphenyl structures tend not to display absorbance maxima within the 290 – 750 nm range. Characteristic absorbance maximum (λ_{max}) and molar extinction coefficients (ε) for three compounds that were identified as components in PEB Bottoms are shown below. Other constituents in PEB Bottoms would have absorbance maxima and extinction coefficients in the range of those chemicals.

Table 8. Characteristic Absorbance Maxima (λ_{max}) and Associated Molar Absorptivities (ε) of Representative Hydrocarbons of PEB Bottoms

Hydrocarbon	λ below 290nm		λ above 290nm	
	λ_{max}	ε	λ_{max}	ε
Cyclohexylbenzene	260	200	--	--
Diphenylmethane	260	470	--	--
1,2-diphenylethane	214	13,300	295	3000

Data from NIST Chemistry WebBook 2003 [http://webbook.nist.gov/chemistry]

Overall, PEB Bottoms will not demonstrate a significant extent of degradation resulting from direct photolysis.

Atmospheric Oxidation (Indirect photodegradation) [Robust Summary, Appendix 2 p. 41]

Atmospheric oxidation as a result of hydroxy radical attack is not direct photochemical degradation but an indirect degradation process. The rate at which an organic compound reacts with OH-radicals is a direct measure of its atmospheric persistence. The AOPWIN version 1.90 computer program [subroutine of EPIWIN 3.12, US EPA, 2000] was used here to estimate the rate constants

for OH- radical reactions of representative organic constituents of PEB Bottoms that are then used to calculate atmospheric half-lives for these constituents as shown below. PEB Bottoms does not have a specific atmospheric half-life; rather, actual half-life ranges for substances in this stream will vary dependent on their constituent composition. The calculated half-life of components of PEB Bottoms, however suggest that PEB Bottoms' atmospheric half-life would be on the order of approximately 1 day.

Table 9. Hydroxy Radical Photodegradation Half-lives of Representative Hydrocarbons of PEB Bottoms

Substance Constituent	Calculated half-life [day]	OH- Rate Constant (cm^3/molecule-sec)
Diethylbenzene	1.3	8.1×10^{-12}
1,3,5-triethylbenzene	0.32	1.4×10^{-11}
1,2,4-triethylbenzene	0.60	3.3×10^{-11}
Cyclohexylbenzene	0.73	1.8×10^{-11}
Diphenylmethane	1.0	1.1×10^{-11}
1,1'- diphenylethane	0.94	1.1×10^{-11}
1,2-diphenlyethane (bibenzyl)	0.89	1.2×10^{-11}
1,1'- diphenylpropane	0.83	1.3×10^{-11}

2.2.3 Stability in Water [Robust Summary, Appendix 2 pp. 43]

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Harris, 1982b; Neely, 1985). This reaction is referred to as nucleophilic substitution, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because carbon atoms lacks sufficient electronegativity to serve as a good leaving group (i.e., carbon-carbon bonds are too stable to be cleaved by nucleophilic substitution). Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Harris, 1982b; Neely, 1985).

The constituent compounds in PEB Bottoms are hydrocarbons that contain only carbon and hydrogen. Thus, the PEB Bottoms stream is not subject to hydrolysis, and this fate process will not contribute to the degradative loss of chemical constituents in this Class II complex mixture.

2.2.4 Transport between Environmental Compartments [Robust Summary, Appendix 2 p.45]

The EQC level 1 Model Version 2.02 (Trent University, 2003) was used to determine partitioning of representative chemical constituents of PEB Bottoms into different environmental compartments. The EQC model uses chemical-physical properties to quantify a chemical's behavior in an evaluative environment. It calculates the distribution of a fixed quantity of conserved (i.e., non-reacting) chemical, in a closed environment at equilibrium, with no degrading reactions, no advective processes, and no inter-media transport processes (e.g., no wet deposition, or sedimentation). The medium receiving the emission is unimportant, because the chemical is assumed to become instantaneously distributed.

Physicochemical input values (molecular weight, water solubility, vapor pressure, partition coefficient, and melting point) for the EQC model were obtained from the EPIWIN (U.S. EPA,

2000) database. Measured values for input parameters were used when available; otherwise, modelled values were employed.

Table 10. Environmental Distribution as Calculated by EQC Level 1 Fugacity Model of Representative Hydrocarbons of PEB Bottoms

Substance Constituent	Calculated Percent Distribution					
	Air	Water	Soil	Sediment	Susp. Sed.	Biota
Diethylbenzene	79.2	0.6	19.8	0.4	<0.1	<0.1
Cyclohexylbenzene	35.3	1.1	62.2	1.4	<0.1	<0.1
1,3,5-triethylbenzene	99.8	<0.1	0.2	<0.1	<0.1	<0.1
1,2,4-triethylbenzene	75.6	0.2	23.7	0.5	<0.1	<0.1
Diphenylmethane	16.3	6.2	75.8	1.7	<0.1	<0.1
1,1'-diphenylethane	28.5	5.2	64.9	1.4	<0.1	<0.1
1,2-diphenylethane	12.7	1.5	83.8	1.9	<0.1	<0.1
1,1'-diphenylpropane	11.9	2.2	84	1.9	<0.1	<0.1

The partitioning data represent a potential distribution range for constituent hydrocarbon chemicals in PEB Bottoms. These hydrocarbons were calculated to partition either to air or soil depending in large part on the number of ring constituents in the molecule. With the exception of cyclohexylbenzene, alkylbenzene constituents were shown to partition primarily to air and secondarily to soil. Cyclohexylbenzene and biphenyl compounds partitioned primarily to soil and secondarily to air. A small percentage of all compounds (<0.1 to 6.2%) partitions to water or sediment (<2%).

2.2.5 Biodegradation [Robust Summary, Appendix 2 p. 47]

Aerobic degradability was determined using the OECD 301D Closed bottle method. Secondary effluent from a wastewater treatment plant treating primarily domestic wastes was collected and filtered then 70mL was added to 14L of nutrient medium and aerated for 4 days. Bulk test solutions were prepared with PEB Bottoms at 2mg/L nominal concentration, sodium benzoate reference substance at 2mg/L or 8mL of water control and stirred for 30 minutes. Each solution was transferred to 10 BOD [Biochemical Oxygen Demand] bottles that were sealed without any headspace. Bottles were incubated in the dark on an environmental shaker at 20^0C and sampled at 0, 8, 14, 21, and 28 days for dissolved oxygen measurements. Percent biodegradation was calculated as Biochemical Oxygen Demand [BOD] divided by the Theoretical Oxygen Demand [ThOD] x 100. PEB Bottoms showed a maximum of 7.1% biodegradation throughout the 28-day test indicating the PEB Bottoms is not readily biodegradable.

3 HAZARDS TO THE ENVIRONMENT

3.1 Aquatic Effects

Testing was performed on a sample that was a blend of equal volumes of six PEB Bottoms samples from different suppliers. Robust summaries of these studies are provided in Appendix 2 pp 49 –58.

3.1.1 Acute Toxicity to Freshwater Invertebrates [Robust Summary, Appendix 2 p.50]

Groups of *Daphnia magna* were exposed to a negative control, solvent control [0.05mL acetone/L] and PEB Bottoms loading rates of 65, 130, 250, 500 and 1000µg/L as water accommodated fractions (WAFs) and assessed for immobilization for 48 hours, according to OECD method 202, Part 1 (1992). Exposure solutions were renewed at 24 hours using fresh WAFs. Concentrations of PEB Bottoms in WAFs were measured at the beginning, at 24 hr renewal [old and fresh solutions] and at 48hrs [old solutions by gas chromatography with flame ionization detection. Measured concentrations ranged from 83 to 94% of nominal loading rate values. OECD guidelines state that it is acceptable to use nominal values in reporting whenever measured values are within 80% of the nominal values.
Based on nominal WAF loading rates, immobilization values were:

24 hour EC50 > 1000µg/L
48 hour EC50 = 340µg/L
48 hour NOEC = 130µg/L
The 48-hour dose-response slope was 9.7.

The results of this study indicate that PEB Bottoms is very toxic to aquatic invertebrates.

3.1.1.a Chronic Toxicity to Freshwater Invertebrates – Modeled [Non-SIDS Endpoint]

An acute-to-chronic ratio (ACR) was applied to the acute Daphnia EC50 data to calculate a chronic maximum-allowable toxicant concentration (MATC) for a 21-day reproduction study with this species. Kenega (1982) after examining 135 different chemicals, determined that an ACR of 25 or less "appears to be a good tool for predicting the chronic toxicity from the acute toxicity for organic industrial chemicals." When ACR of 25 was applied to the measured Daphnia magna 48-hr EC50 value of 340µg/L, the resulting estimated chronic MATC value was 14µg/L, indicating that PEB Bottoms is very toxic to aquatic invertebrates with potential for long lasting effects.

3.1.2 Acute Toxicity to Freshwater Fish [Robust Summary, Appendix 2 p. 53]

The fathead minnow, *Pimephales promelas*, was exposed to a negative control, solvent control [0.05mL acetone/L] and PEB Bottoms loading rates of 3.3, 6.5, 13, 25, and 50mg/L of water accommodated fractions (WAFs), under static renewal conditions and assessed for survival during a 96 hour exposure duration, according to OECD method 203 (1992). Duplicate test jars contained 5 fish at each dose level and were sealed with no headspace. Fish were transferred to newly prepared WAF solutions at 24, 48 and 72 hours. Concentrations of PEB Bottoms in WAFs were measured in fresh solutions collected at 0 and 72 hours and old solutions at 24 and 96 hours by gas chromatography with flame ionization detection. Measured concentrations ranged from 0.783mg/L, 24% of nominal at 3.3mg/L exposure level to 2.55mg/L, 5% of nominal at 50mg/L exposure level.

96 hour LC50 = 1.65mg/L based on mean measured concentration. [between 13 and 25mg/L nominal]
96 hour NOEC = 1.03mg/L based on mean measured concentration [6.5mg/L nominal]
The 96 hour dose response slope = 14

The results of this study indicate that PEB Bottoms is toxic to freshwater fish.

3.1.3 Toxicity to Aquatic Plants (Freshwater algae) [Robust Summary, Appendix 2 p. 56]

The freshwater algae, *Pseudokirchneriella subcapitata*, was exposed to a negative control, solvent control [0.05mL acetone/L and PEB BOTTOMS loading rates of 65, 130, 250, 500 and 1000µg/L as water accommodated fractions (WAFs) and assessed for growth inhibition (biomass) and growth rate, according to OECD method 201. The WAFs were prepared in freshwater algal nutrient medium and algae were exposed under static conditions in sealed vessels for 72 hours. Concentrations of PEB Bottoms in WAFs were measured at the beginning and end of the test by gas chromatography. Mean measured concentrations ranged from 68 to 80% of the nominal loading rate values. The area under the curve and growth rate were taken as indices of algal growth and were calculated for each treatment group using cell densities determined at 24, 48 and 72 hours.

Biomass: 72 hour EbC50 = 320µg/L nominal [251µg/L mean measured concentration]
Growth: 72 hour ErC50 = 640µg/L nominal [485µg/L mean measured concentration]
72 hour NOEC = 130µg/L nominal [95.9µg/L mean measured concentration]

The results of this study indicate that PEB Bottoms is very toxic to aquatic plants.

3.2 Terrestrial Effects [Non-HPV SIDS endpoint]

No studies of terrestrial effects are reported for PEB Bottoms.

3.3 Initial Assessment for the Environment

The environmental fate of PEB Bottoms has been determined by evaluating data developed for individual compounds identified as components of PEB Bottoms. These constituent hydrocarbons have a very low potential to hydrolyze and do not degrade directly due to a minimal capacity to absorb appreciable light energy above 290nm. However atmospheric oxidation constitutes a significant route of degradation. Calculation of atmospheric half-lives of 8 representative constituent chemicals identified a range of 0.32 to 1.3 days as a result of indirect hydrolysis by hydroxy radical attack, suggesting that PEB Bottoms' atmospheric half-life would be on the order of approximately 1 day. Fugacity modelling demonstrated that constituent hydrocarbons in PEB Bottoms partition either into air or soil at percentages depending in large part on the number of ring constituents in the molecule, with a small percentage of any compound partitioning into water or sediment. PEB Bottoms is not readily biodegradable, demonstrating 7.1% degradation over a 28-day test period. Toxicity to aquatic species exposed to water accommodated fractions of PEB Bottoms occurs within a similar range of concentrations over 48-96 hours: *Daphnia* 48 hr. EC50 = 340µg/L, Alga 72 hr EbC50 = 320µg/L and minnow 96 hr EC50 = 1.65mg/L (1650µg/L). Using the acute toxicity hazard to *Daphnia* to estimate a chronic toxicity value of 14µg/L for this species, PEB Bottoms was determined to pose a chronic toxicity hazard to invertebrates as well. These results indicate that PEB Bottoms is toxic to very toxic to aquatic life and that *Daphnia* and algae may be somewhat more sensitive to PEB Bottoms WAF exposure than freshwater fish. These data are sufficient to classify the ecotoxicity hazard from PEB Bottoms.

4 HUMAN HEALTH HAZARDS

4.1 Effects on Human Health

Toxicity data have been developed for PEB Bottoms to meet the Tier 1 specifications of the HPV Testing Program. With exception of the acute data, testing was performed on a sample that was a blend of equal volumes of six PEB Bottoms samples from different suppliers. The PEB Bottoms

for the acute tests was a sample of one sponsor's PEB Bottoms product. Robust summaries of these studies are provided in Appendix 2, pp. 59-72.

4.1.1 Acute Toxicity

Studies in Animals

Acute Oral, Rats [Robust Summary, Appendix 2 p. 60]

LD50 > 5.0g/kg

Fischer 344 rats were treated with a single dose of PEB Bottoms by gastric intubation and observed for 9 days. No mortality and no adverse effects on body weight were observed. Some clinical signs were reported intermittently. No adverse effects were seen at gross necropsy at study termination.

Acute Dermal, Rats [Robust Summary, Appendix 2 p. 61]

Acute toxicity >2.0g/kg after application for 5 consecutive days.

The backs of Fischer 344 rats were shaved prior to treatment and each rat was fitted with an Elizabethan collar to prevent ingestion. Test concentrations of PEB Bottoms at 2g/kg undiluted 100% PEB Bottoms or 1g/kg PEB Bottoms as 50% in light paraffin oil were applied for 6 hours each day over a 5-day period. No mortality occurred. Decreased body weight, clinical signs and some skin irritation were seen.

Conclusion

This test material was a sample of PEB Bottoms from one sponsor's facility but is considered representative of the acute toxicity potential of PEB Bottoms. PEB Bottoms demonstrated no mortality and minimal acute toxicity by the oral or dermal routes of exposure.

4.1.2 Irritation [Non-SIDS endpoint] [Robust Summary, Appendix 2 p. 61]

There are no reports of skin or eye irritation studies conducted for PEB Bottoms. Skin irritation effects, however, were observed on the backs of rats that were repeatedly exposed to a neat and diluted PEB Bottoms. The skin effects included erythema, barely perceptible in 1.0g/kg/day rats, and slight to well defined in 2.0g/kg/day rats. Barely perceptible edema, and focal thickening of the skin at the point of application were also seen in 2.0g/kg/day rats.

4.1.3 Sensitization [Non- SIDS endpoint]

There are no reports of skin sensitization studies conducted for PEB Bottoms.

4.1.4 Repeated Dose Toxicity [Robust Summary, Appendix 2 p. 63]

Studies in Animals: Oral

PEB Bottoms was tested in a Combined 28 day repeated dose toxicity study with neurobehavioral endpoints and reproductive/developmental screening according to OECD method 422 (1996). Sprague Dawley rats (12M, 12F per group) were given PEB Bottoms in corn oil at doses of 0, 20, 80 and 320mg/kg once daily by oral gavage, 7 days/week. Males were treated from 14 days prior to mating to 1 day prior to sacrifice or on the day of sacrifice for males assessed for neurobehavioral parameters, for a total of 37-39 days. Females were treated from 14 days prior to mating through gestation to lactation day (LD) 3 or 4 if assessed for neurobehavioral parameters for a total of 39 (non-mated females) to 52 doses. Animals were housed in individual stainless steel wire mesh cages until mating then paired 1:1 in the male's home cage. At gestation day (GD) 0, females were transferred to plastic boxes with ground corncob bedding as nesting material. Females remained

housed in these boxes until sacrifice at lactation day (LD) 4 [Further information on reproductive toxicity is summarized in Section 4.1.7]. Dosing solutions were prepared weekly and evaluated for homogeneity, resuspension homogeneity, and stability. PEB Bottoms test formulations contained the appropriate concentrations and were homogeneous and stable for at least 8 days.

All rats survived to scheduled necropsy. Clinical signs included hair loss on ventral abdomen or hind limbs, and clear or red material on body surfaces one hour after dosing seen in 92% of rats in the 320mg/kg/day group and 33% of males and 75% of females in 80mg/kg/day rats. Clear or red material was considered to be due to potential taste aversion to the test article and not a sign of toxicity. The finding seen shortly after dosing did not persist to the next observation point. No clinical findings were observed in 20mg/kg/day rats. Mean body weights in males were 13% and 8% lower and weight gain was 42% and 26% less than controls by the end of the exposure period in the 320 and 80mg/kg/day groups, respectively. Changes in food consumption varied weekly but were only statistically significantly decreased as g/animal/day during the second week of exposure in the 320mg/kg/day group males. Female body weights were not affected prior to gestation; thereafter the 320mg/kg/day pregnant animals had a 10% lower mean body weight at GD20 and a 21% less weight gain over GD0-20. No effects were seen in 80 and 20mg/kg/day females. No significant PEB Bottoms related effects on FOB parameters or locomotor activity were observed in males tested during study wk 5 or females on LD 4. No hematology findings were observed other than a decrease in mean absolute and/or % eosinophils in 80mg/kg/day males [78% and 56% of control values, respectively] and 320mg/kg/day animals of both sexes [approximately 50% of both parameters]. Serum chemistry parameters were unaffected by treatment at all dose levels. Increases of 10% in mean and 20-25% relative kidney weights in 80 and 320mg/kg/day males and increased mean [20%] and relative liver weights [27-37%] in 320mg/kg day rats of both sexes correlated with microscopic findings [mineralization, multifocal deposits and irregular basophilic material in male kidneys, and hepatocellular hypertrophy, respectively]. Increased thyroid gland weights of 10-15% compared to controls in both sexes and decreased thymus weights of 23% in females in the 320mg/kg/day group correlated with microscopic changes [follicular cell hypertrophy in the thyroid, and thymic atrophy in females, respectively] but were not seen in the 80 and 20mg/kg/day animals.

Conclusion

Systemic NOAEL = 20mg/kg/day
Systemic LOAEL = 80mg/kg/day [decreased body wt and/or food consumption, organ wt changes and microscopic findings in 320mg/kg/day organs]

PEB Bottoms induced adult systemic toxicity expressed as decrements in body weight and body weight gain, some decreased food consumption and changes in organ weights at 80 and 320mg/kg/day groups with correlative microscopic findings in 320mg/kg/day animals. No adverse effects were seen on neurobehavioral parameters.

4.1.5 Genetic Toxicity [Robust Summary, Appendix 2 pp. 68-72]

In vivo Studies

There is no *in vivo* genetic toxicity information reported for PEB Bottoms.

In vitro Studies

Bacterial Reverse Mutation Assay for gene mutation [Robust Summary, Appendix 2 p.68]

PEB Bottoms was tested with *Salmonella typhimurium* [TA 98, 100, 1535, 1537] and *Escherichia coli* WP2uvrA in a plate incorporation assay with and without metabolic activation from rat liver

homogenate according to OECD method 471 (1998). Dose concentrations ranged from 1.5 to 5000µg/plate of PEB Bottoms solubilized in EtOH. Initial and repeat trials were performed to verify results.

PEB Bottoms induced a positive repeatable mutagenic response in *Salmonella typhimurium* TA 100 with metabolic activation. The increase did not exceed 2.9 fold of negative controls in any trial. No other strain of *Salmonella* or *E. coli* demonstrated significant mutagenic activity. PEB Bottoms is a bacterial mutagen in this test system.

***In vitro* Chromosome Aberration Assay [Robust Summary, Appendix 2 p. 70]**

Chinese Hamster Ovary (CHO) cells were exposed to PEB Bottoms solubilized in EtOH over a concentration range of 3.13 to 150µg/ml in a chromosome aberration assay; analyzed doses were 0, 6.25, 12.5 and 25.0µg/ml with and without metabolic activation from rat liver homogenate according to OECD method 473 (1998). The highest dose level selected for analysis of chromosome aberrations was the dose that induced at least 50% toxicity as measured by mitotic inhibition relative to solvent controls with a sufficient number of scorable metaphase cells. Initial and repeat trials were performed to verify results.

No biologically significant increases in structural or numerical aberrations were observed in chromosomes at any dose levels in any exposure regimens with or without metabolic activation. PEB Bottoms is not clastogenic to mammalian cells in culture.

Conclusion

PEB Bottoms induces gene mutation in bacterial cells with metabolic activation but does not induce cytogenetic damage in mammalian cells in culture.

4.1.6 Carcinogenicity [Non-SIDS endpoint]

There is no carcinogenicity information reported for PEB Bottoms

4.1.7 Toxicity for Reproduction

Effects on Fertility and Developmental Toxicity [Robust Summary, Appendix 2 p. 68]

PEB Bottoms was tested in a Combined 28 day repeated dose toxicity study with neurobehavioral endpoints and reproductive/developmental screening according to OECD method 422 (1996). Sprague Dawley rats (12M, 12F per group) were given PEB Bottoms in corn oil at doses of 0, 20, 80 and 320mg/kg once daily by oral gavage, 7 days/week as reported earlier in Section 3.1.4. On gestation day (GD) 0, presumed-pregnant females were transferred to plastic boxes with ground corncob bedding as nesting material. Females remained housed in these boxes until sacrifice at lactation day (LD) 4.

No effects on body weight or food consumption were seen in females prior to gestation; thereafter the 320mg/kg/day pregnant animals had a 10% lower mean body weight at GD20 and 21% less weight gain over GD0-20. During the four days of lactation, mean body weight gain were reduced by 17% compared to controls and the LD 4 weight was 8% less than controls in 320mg/kg/day females. No effects were observed in 80 or 20mg/kg/day group females. Mean food consumption in all groups of females during gestation and lactation were comparable to controls. Pregnant rats were observed daily for parturition and gestation length was calculated from the date at which parturition began. On postnatal day 0, pups were sexed and examined for malformations. No adverse effects were observed on male or female mating or fertility. Mean gestation length in the 320mg/kg/day group (22.6 days) was increased [$p<0.01$] compared to controls (21.6 days). At

necropsy the mean number of implantation sites was decreased by 9% in both 80 and 320mg/kg/day groups and the mean number of unaccounted for sites was increased in the 320mg/kg/day group (2.2 pups/dam compared to 1.0 pup/dam in controls). The mean number of pups born and live litter sizes on postnatal day 0 were reduced in the 80 and 320mg/kg/day groups. Values in the 80mg/kg/day group were 89% of control for mean pups born and live litter size and for the 320mg/kg/day group were 81% mean pups born and 79% mean live litter size of control values. However none of these findings were statistically significant. Among the F1 offspring, no PEB Bottoms related effect on the percentage of males at birth or postnatal survival was noted at any dose level. The general physical condition and mean pup body weights were unaffected by PEB Bottoms treatment of parental animals at any dose level. There were no PEB Bottoms-related findings on pups found dead or at scheduled necropsy on postnatal day 4.

Conclusion

Reproductive NOAEL = 20mg/kg/day
Reproductive LOAEL = 80mg/kg/day [extended gestation, decreased number of implantations and pups born, and decreased live litter size].

Repeated exposure of rats to PEB Bottoms produced indications of reproductive toxicity. Reproductive changes induced by PEB Bottoms included extended mean gestation length in 320mg/kg/day females and observed decreases in implantation sites, numbers of pups born and live litter size in 80 and 320mg/kg/day groups and increased unaccounted for sites at 320mg/kg/day. Although the changes in implantation sites, unaccounted for sites, pups born and live litter size were not statistically significant, these dose-related occurrences were considered biologically significant for this screening test.

Neonatal toxicity NOAEL = 320mg/kg/day

4.2 Initial Assessment for Human Health

PEB Bottoms induced no mortality and minimal acute toxicity by the oral or dermal routes of exposure in rats. No standard skin irritation studies have been conducted for PEB Bottoms, however some skin irritation [erythema and slight edema] was reported in rats following repeated exposure to PEB Bottoms in a dermal toxicity study. PEB Bottoms induced gene mutation in bacterial cells but did not cause cytogenetic damage in mammalian cells in culture. Treatment with PEB Bottoms at oral doses of 80 or 320mg/kg/day for 37 days (males) or up to 52 days (females) induced adult systemic toxicity expressed as decreased body weight and body weight gain, and changes in some organ weights, primarily kidney (male) and liver with comparable microscopic findings. PEB Bottoms did not cause adverse effects on neurobehavioral parameters. Male and female fertility were comparable to controls although the mean gestation duration was increased in high dose females. Adverse trends in toxicity were seen for some reproductive parameters [decreased implantation sites, number of pups born and live litter size, and increased unaccounted for sites] but were not statistically significant. Postnatal survival, body weight and physical condition of F1 offspring were unaffected by PEB Bottoms treatment of parental animals at any dose level. These results suggest the possibility of PEB Bottoms-induced reproductive effects *in utero* but no adverse PEB Bottoms effects on neonatal animals.

5 PROGRAM SUMMARY AND RECOMMENDATIONS

PEB Bottoms is a complex aromatic hydrocarbon stream that is a co-product of ethylbenzene manufacture. Ethylbenzene is produced by the alkylation of benzene with ethylene. In addition to the production of ethylbenzene, there are side reactions to produce di-, tri- and polyethylbenzene as

well as butylbenzene and other alkylaromatics. After removal of ethylbenzene from the reaction product, the remaining stream is separated into a diethylbenzene-rich distillate stream and a Bottoms stream described as benzene, ethylenated, residues or Polyethylbenzene Bottoms. The composition of this Bottoms stream varies with the manufacturer and processing. The PEB Bottoms sample used in this HPV testing program was a blend of equal volumes of 6 PEB Bottoms samples from 6 different suppliers. The material is a liquid with low vapor pressure under ambient conditions. Likely routes of exposure are inhalation and accidental dermal contact. Workplace exposure is limited because of the low vapor pressure of the stream and because production occurs primarily in a closed system. When shipped, the material is transported in tank cars or trucks to relatively few locations. The general population is unlikely to be exposed to PEB Bottoms because there are no direct consumer uses for this material. Polyethylbenzene Bottoms is a volatile organic compound (VOC) and is subject to USEPA and state regulations that limit VOC emissions. Emissions of PEB Bottoms are relatively low from manufacturing and use facilities. Facilities that produce and use PEB Bottoms are also typically subject to state operating permits and regulations that further limit VOC emissions.

Physicochemical, Environmental and Aquatic Endpoints: Physical chemical properties, biodegradation and aquatic toxicity studies were performed using the PEB Bottoms blended sample. For environmental endpoints, measured data on components present in PEB Bottoms have been evaluated. Where measured data do not exist, calculated data have been developed using EPIWIN© computer models described by EPA. Transport between environmental compartments was modelled using the EQC Level 1 Fugacity Model, an appropriate model for complex mixtures. Constituent hydrocarbons have a very low potential to hydrolyze and do not degrade directly due to a minimal capacity to absorb appreciable light energy above 290nm. However atmospheric oxidation constitutes a significant route of degradation. Calculation of atmospheric half-lives of 8 representative constituent chemicals identified a range of 0.32 to 1.3 days as a result of indirect hydrolysis by hydroxy radical attack. Fugacity modelling demonstrated that constituent hydrocarbons in PEB Bottoms partition either into air or soil at percentages depending in large part on the number of ring constituents in the molecule with only a small percentage of any compound partitioning into water or sediment. PEB Bottoms is not readily biodegradable. Toxicity to aquatic species exposed to water accommodated fractions of PEB Bottoms occurs within a similar range of concentrations over 48-96 hours: *Daphnia* 48 hr. EC50 = 340µg/L, Alga 72 hr EbC50 = 320µg/L and minnow 96 hr EC50 = 1.65mg/L (1650µg/L). These results indicate that PEB Bottoms is toxic to very toxic to aquatic life and that *Daphnia* and algae may be somewhat more sensitive to PEB Bottoms WAF exposure than freshwater fish. Using the acute toxicity hazard to *Daphnia* to estimate a chronic toxicity value, PEB Bottoms was determined to pose a chronic toxicity hazard to invertebrates as well. However PEB Bottoms is not generally used in emissive applications, and thus would not be expected to enter the environment.

Human Health Effects: With the exception of the acute toxicity studies, all mammalian toxicity studies were performed with the PEB Bottoms blended sample. PEB Bottoms did not cause deaths of rats and was minimally toxic by the oral and dermal routes although some skin irritation was seen in the dermal study. PEB Bottoms induced gene mutation in bacteria but did not induce chromosome aberrations in mammalian cells in culture. Effects in the OECD 422 Combined 28 day Repeated Dose Toxicity Study with Reproductive/Developmental Screening by the oral route included decreased adult body weight and body weight gain, decreased food consumption, increased kidney (males only), liver and thyroid weights, and decreased thymus weights which correlated with microscopic changes. Neurobehavioral parameters were not affected by PEB Bottoms treatment. Male and female fertility was comparable to control values although mean gestation duration was increased in high dose females. Adverse trends in some reproductive

parameters suggested the possibility of PEB Bottoms-induced reproductive effects but no neonatal toxicity affecting offspring survival, physical condition or body weights occurred.

The body of data provided here fulfils the Tier 1 testing recommendations of the HPV program. In consideration of the controlled production and usage, and limited exposure potential of PEB Bottoms, the screening level information provided in this report is adequate to characterize the potential hazard of this substance.

REFERENCES

ASTM Method D1015-99. Standard Test Method for Freezing Points of High Purity Hydrocarbons. 11pp.

Benoit F.M. et al. 1978. Int J Environ Anal Chem 6: 277-87.

BP Amoco Company. 2000 Unpublished Report for American Chemistry Council Ethylbenzene Panel (CMA Reference No. EB-60-RES-HPV-BP Amoco) June 7, 2000. BP Amoco Technology Center Naperville, IL.

Coleman E.C. et al., 1981. J Agric Food Chem 29: 423-8.

Fielding M. et al. 1981. Micropollutants in Drinking Water. TR-159. Medmenham England: Water Res Center.

Harris, J.C. 1982a. Rate of Aqueous Photolysis, Chapter 8 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Harris, J.C. 1982b. "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

Karasek F.W. et al., 1987. Anal Chem 59: 1027-31.

Kenega, E.E. 1982. Predictability of chronic toxicity from acute toxicity of chemicals in fish and aquatic invertebrates. Environ Toxicol Chem 1: 347-358.

Kool H.J. et al., 1982. Crit Rev Environ Control 12: 307-57.

Konasewich D. et al., 1978. Status Report on Organic and Heavy Metal Contaminants in the Lakes Erie, Michigan, Huron and Superior Basins. Great Lakes Water Quality Board.

National Institute of Standards and Technology (NIST). 2003. NIST Standard Reference Database Number 69 – March 2003 Release. NIST Chemistry WebBook. [http://webbook.nist.gov/chemistry].

Neely W. B. 1985. “Hydrolysis”, Chapter 7 in: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I. 173. CRC Press, Boca Raton, FL, USA.

Shackelford W.M. et al. 1980. Analyt Chim Acta 146: 15-27.

Trent University. 2003. EQC Fugacity-Based EQC-Equilibrium Criterion Model. Canadian Environmental Modeling Centre, Trent University, Peterborough, Ontario (http://www.trentu.ca/cemc/).

US EPA 2000. EPIWIN API (Estimation Program Interface) suite, version 3.12. Subroutine MPBPWIN, V. 1.41. US Environmental Protection Agency, OPPT, Washington, DC

US EPA Toxics Release Inventory (TRI) [http://www.epa.gov/tri.]

APPENDIX 1

CHARACTERIZATION REPORT FOR TS-16672 (POLYETHYLBENZENE BOTTOMS BLEND)

Component	Wt %
diethylbenzene	0.01
1,3,5-triethylbenzene	6.20
1,2,4-triethylbenzene	7.23
cyclohexylbenzene	0.66
diphenylmethane	20.45
1,1'-diphenylethane	25.42
1,2-diphenylethane (bibenzyl)	7.98
1,1'-diphenylpropane	2.42

The Polyethylbenzene Bottoms stream blend (PEB Bottoms Blend) was comprised of equal volumes of polyethylbenzene sample from six sources. Pertinent information from each of these sources was as follows:

Source	Date Received	ABC reference number(s)
Dow Chemical	June 11, 2004	TS-16578, TS-16579
BP Amoco	June 23, 2004	TS-16612
Lyondell Chemical	June 24, 2004	TS-16613
Nova Chemical	June 25, 2004	TS-16619
Chevron Phillips Chemical	June 29, 2004	TS-16622
Atofina Petrochemicals	June 30, 2004	TS-16624, TS-16625

The PEB Bottoms blend was prepared on July 13, 2004, by combining 1.5-L volumes from each source into a 9-L glass carboy. The mixed contents in the carboy were transferred to 10 appropriately labeled 1-L amber bottles. The PEB Bottoms blend was stored at room temperature and assigned reference number TS-16672.

The blended material was analytically characterized by gas chromatography/mass spectrometry.

APPENDIX 2

Robust Summaries
For
Polyethylbenzene Bottoms

TABLE OF CONTENTS

Physico-Chemical Properties

Environmental Endpoints

Aquatic Toxicity

Human Health Hazards

1.3 PHYSICO-CHEMICAL PROPERTIES

1.3.1 Freezing Point

Test Substance:	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	OECD #102 (1995)
Type (test type):	ASTM D 1015-99
GLP:	No
Year (study performed):	2005
Test Conditions:	The PEB sample was a blend of equal volumes of six PEB samples from different suppliers. The PEB sample was prepared at ABC Laboratories, Inc., Columbia, MO. The freezing point testing was performed at Harris Testing Laboratories, Houston, TX. The freezing point of the test substance was determined in triplicate following ASTM method D 1015-99. As the test substance was cooled, the temperature was recorded every fifteen seconds. A temperature versus time plot was prepared for each replicate determination. The freezing point was determined from the equilibrium portion of the freezing curve.
Results:	Analysis of the equilibrium portion of each replicate resulted in a test substance freezing point of –58.8°C. The results are summarized below: Replicate / Freezing Temperature (°C) 1 / -58.8 2 / -58.8 3 / -58.8 Mean / -58.8 ± 0.0
Conclusion: (Laboratory contractor)	The freezing point of PEB was determined to be –58.8 ± 0.0°C.
Reliability:	**2.** Reliable with restrictions. The testing laboratory is a reputable analytic laboratory but does not meet all procedures specified under GLP.
Reference:	Determination of Freezing Point for a Polyethylbenzene Bottoms Stream (PEB) Blend. 2005. Huntley, K. ABC Study No. 49022, ABC Laboratories, Inc. Columbia, MO. Sponsor American Chemistry Council, Arlington, VA ASTM Method D1015-99, Standard Test Method for Freezing Points of High Purity Hydrocarbons. 11pp.
Other (source) Last changed	1/31/06

1.3.2 Boiling Point -measured

<table>
<tr><td>Test Substance:</td><td>Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.</td></tr>
<tr><td>Method/Guideline:</td><td>OECD #103 (1995)</td></tr>
<tr><td>Type (test type):</td><td>Automated system, improved Siwoboloff method</td></tr>
<tr><td>GLP:</td><td>Yes</td></tr>
<tr><td>Year (study performed):</td><td>2005</td></tr>
<tr><td>Test Conditions:</td><td>The PEB sample was a blend of equal volumes of six PEB samples from different suppliers. A Mettler FP900 Thermosystem consisting of a Mettler FP81HT MBC Cell attached to a Mettler FP90 Central processor was used to determine the boiling point of the test substance. A Princo mercury barometer was used for barometric pressure measurements. To verify that the instrument was working properly, the boiling point of ethyl alcohol was determined to be 78.5+0.1^{0}C, very similar to the CRC Handbook value of 78.5^{0}C.
PEB was added to a boiling point tube to a height of 15-18 mm. A boiling capillary was inserted into the boiling point tube until the capillary rested on the base of the tube. The tube was analyzed by inserting the tube into the center slot of the instrument. This sample was analyzed starting at 258ºC and increasing at +0.2ºC/minute until the boiling point was reached. The boiling point recorded was calculated by the instrument using the actual boiling temperatures and barometric pressure (99.2 kPa) measurements. The boiling point values were corrected to standard pressure (101.325 kPa) automatically by the instrument.</td></tr>
<tr><td>Results:</td><td>The boiling point of PEB was determined to be 262.2 ± 0.3°C (535.4 K) as shown in the following table:
<table>
<tr><th>Replicate</th><th>Boiling Temperature (°C)</th><th>Boiling Point (°C)</th></tr>
<tr><td>1</td><td>260.9</td><td>261.9</td></tr>
<tr><td>2</td><td>261.3</td><td>262.3</td></tr>
<tr><td>3</td><td>261.5</td><td>262.5</td></tr>
<tr><td></td><td>Mean</td><td>262.2 ± 0.3 (535.4 K)</td></tr>
</table>
There was no indication of test substance decomposition.</td></tr>
<tr><td>Conclusion:
(Laboratory contractor)</td><td>The boiling point of PEB was determined to be 262.2 ± 0.3°C (535.4 K).</td></tr>
<tr><td>Reliability:</td><td>2. Reliable with restrictions. Since PEB is a complex mixture of hydrocarbons, a boiling point range was modeled using EPIWIN computer model, V3.12 (U.S. EPA, 2000). For the principal chemical components in PEB, modeled boiling point values ranged from 191 to 291°C.</td></tr>
<tr><td>Reference:</td><td>Determination of Boiling Point for a Polyethylbenzene Bottoms Stream (PEB) Blend. 2005. Huntley, K. ABC Study No. 49023, ABC Laboratories, Inc. Columbia, MO. Sponsor American Chemistry Council, Arlington, VA
U.S. EPA. 2000. API (Estimation programs interface) suite, V 3.12, subroutine MPBPWIN, V 1.41. US Environmental Protection Agency, Office of pollution prevention and toxics, Washington DC.</td></tr>
</table>

Other (source) Last changed	1/31/06

1.3.2 Boiling Point-modeled

Test Substance	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline	EPIWIN computer model; V3.12 (U.S. EPA, 2000). This model calculates boiling point based on the method of Stein and Brown (J. Chem. Inf. Comput. Sci. 34, 1994).
GLP	No
Year (study performed)	Not Applicable
Results: Boiling Point Value	Calculated and measured boiling point data for representative constituents of PEB are listed below. The data identify a potential boiling point range for substances represented by CAS RN. 68987-42-8. **Boiling Point, °C** **Chemical Name** — **Measured** — **Modeled** Diethylbenzene — 181.0 — 191 Cyclohexylbenzene — 240.1 — 238 1,2,5-triethylbenzene — 215.9 — 230 1,2,4-triethylbenzene — 218.0 — 230 Diphenylmethane — 265.0 — 269 1,1-diphenylethane — 272.6 — 276 1,2-diphenylethane — 284.0 — 285 1,1'-diphenylpropane — 281.6 — 291 Measured values for the respective compounds were cited by the EPIWIN experimental database. Not Applicable Not Applicable Values given above represent a range of estimated and measured boiling point determinations for the principal chemical components characterized in PEB (CAS RN. 68987-42-8).
Pressure, units Decomposition Remarks	
Conclusions	For the principal chemical components characterized in Polyethylbenzene Bottoms (CAS No. 68987-42-8), modeled boiling point values ranged from 191 to 291°C. Measured boiling point values for these constituents cited in EPIWIN's experimental database ranged from 181 to 284 °C.
Reliability	**1.** Reliable without restrictions. This robust summary presents measured and modeled boiling point ranges based on a characterized PEB stream.
References	U.S. EPA. 2000. API (Estimation programs interface) suite, V 3.12, subroutine MPBPWIN, V 1.41. US Environmental Protection Agency, Office of pollution prevention and toxics, Washington DC.
Other (source) Last changed	 1/31/06

1.3.3 Vapor Pressure

Test Substance:	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	OECD #104 (1995)
Type (test type):	Vapor Pressure determination
GLP:	Yes
Year (study performed):	2005
Test Conditions:	The PEB sample was a blend of equal volumes of six PEB samples from different suppliers. Reagent water had been purified using a Millipore Milli-Q Purification system. Thermometer was NIST-verified. The vapor pressure apparatus was a Terranova model 908A dual capacitance diaphragm gauge controller, Baratron pressure transducer, Franklin electric vacuum pump model 4401007400, and 100-mL long-necked, round bottom flasks with sidearm. Atmospheric pressure was checked prior to use each day using a NOVA mercury barometer. Verification of the vapor pressure testing apparatus was performed once a year by determining the vapor pressure of water at 20^0C in triplicate. The vapor pressure of water was determined to be 17.4 ± 0.1 torr (2320Pa) within 0.4% of reported literature values. At the initiation of the study, approximately 25ml PEB was added to the test flask. The sample was degassed at reduced temperature by supercooling using an acetone/dry ice bath. The flask valve was opened for several minutes to remove any liberated air, then was closed. Following 30 minutes of immersion in the water bath set at 10°C, the vapor pressure reading was recorded. The temperature of the waterbath was adjusted to 20 and 30°C. After allowing the sample to equilibrate to each test temperature for 30 minutes, the vapor pressure value was recorded. The temperature of the waterbath at each test temperature was verified using a thermometer. This procedure was repeated for a second replicate determination.
Results:	The vapor pressure of PEB was determined to be less than 90 Pa at 10, 20, and 30°C, respectively. All pressure readings at 10, 20, and 30°C were less than 0.7 torr (90 Pa). Target Temp. (°C) / Replicate Number / Temp. Reading (°C) / Vapor Pressure (torr)[a] / Vapor Pressure (Pa)[1] 10 / 1 / 10.0 / < 0.7 / < 90 2 / 10.0 / < 0.7 / < 90 20 / 1 / 20.0 / < 0.7 / < 90 2 / 20.0 / < 0.7 / < 90 30 / 1 / 30.1 / < 0.7 / < 90 2 / 30.0 / < 0.7 / < 90 [a]1 torr = 1.33322 x 10^2 Pa The vapor pressure was reported as less than 10^2 Pa at each of the temperatures evaluated.
Conclusion: (Laboratory contractor)	The vapor pressure of PEB was determined to be less than 10^2 Pa at 10, 20, and 30°C, respectively.
Reliability:	**1.** Reliable without restrictions.

Reference:	Determination of Vapor Pressure for a Polyethylbenzene Bottoms Stream (PEB) Blend. 2005. Huntley, K. ABC Study No. 49024, ABC Laboratories, Inc. Columbia, MO. Sponsor American Chemistry Council, Arlington, VA
Other (source) Last changed	1/31/06

1.3.4 Partition Coefficient

Test Substance	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/guideline	OECD Method 117, HPLC method (2004)
GLP	Yes
Year (study performed)	2005
Test Conditions:	The PEB sample was a blend of equal volumes of six PEB samples from different suppliers. The HPLC system included a Phenomenex Primesphere 5 C18 HC column, 250 mm x 4.6 mm id, with a mobile phase of 75:25 acetonitrile:reagent water at a flow rate of 1.0 mL/min. Fifty microliter samples of a 11.5 μg/mL solution of PEB in mobile phase were injected, and the emergence of the material was observed using UV detection (λ = 210 nm). Eight reference compounds were used to generate the linear relationship between log k (k = capacity factor) and log Pow. Using the HPLC retention time for the peak of the test substance, the log k was determined, and the log Pow value was calculated using a linear equation developed from the reference compounds. HPLC analysis of the test substance resulted in multiple peaks, thirteen of which were attributed to PEB. The log P_{ow} values for each of the peaks of the test substance were determined by substituting their experimentally determined log k values into the equation derived from the log k versus log P_{ow} graph constructed from the reference standards.
Results: Log Pow Temperature, °C Remarks	 4.08 to 6.01 20 °C The cited values represent a range of Log Pow values for components making up the complex mixture of PEB.
Conclusion: (Laboratory contractor)	Log Pow = 4.08 to 6.01
Reliability:	**1.** Reliable without restrictions.
Reference	Serak, Kelda. 2005. Determination of n-Octanol/Water Partition Coefficient(s) for Polyethylbenzene Bottoms Stream Blend (PEB Blend) by High Performance Liquid Chromatography (HPLC). ABC Laboratories, Inc., Columbia, MO. Sponsor: American Chemistry Council, Arlington, VA
Other (source) Last changed	 1/31/06

1.3.5 Water Solubility

Test Substance	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline	OECD Method 105 (1995)
GLP	Yes
Year (study performed)	2005
Test Conditions:	The PEB sample was a blend of equal volumes of six PEB samples from different suppliers. Water solubility was measured using the shake flask method described in OECD guideline 105 and the Official Journal of the European Communities (OJ). Test samples were prepared by adding 3 mL of PEB to each of three, 40-mL plastic centrifuge tubes. Thirty-three milliliters of reagent water was added to each tube. The samples were capped and placed on an orbital shaker water bath set at 30 °C and agitated. One replicate was removed from the shaker after approximately 24, 48, and 72 hours and placed on a shaker at 20 °C. Five days after placing the first sample on the shaker at 20 °C, the three samples were removed. Samples were centrifuged for 30 minutes at 20,000 rpm (44,720 x g) and 20 °C. The aqueous layers were removed to 40-mL scintillation vials using glass syringes with removable needles. Twenty mL of each sample was extracted and analyzed by gas chromatography. Analyses were done using gas chromatography with a flame ionization detector. Responses of standards and samples were calculated as the sum of the responses from six marker peaks within the PEB chromatogram.
Results Value, at temperature °C Description pH value pKa value at 25 °C Remarks	 29.5 ± 1.4 mg/L at 20 ± 0.5°C N/A 8.04, 7.10, and 7.24 at the 24-, 48-, and 72-hour sampling points, respectively N/A The solubility measurements at 48 and 96 hours averaged 30.7 mg/L and 28.4 mg/L, respectively. The final water solubility value was the overall mean of the 48 and 96 hour sample determinations.
Conclusion: (Laboratory contractor)	Water solubility was 29.5 ± 1.4 mg/L at 20 ± 0.5°C
Reliability:	**1.** Reliable without restrictions.
Reference	Serak, Kelda. 2005. "Determination of Water Solubility for Polyethylbenzene Bottoms Stream Blend (PEB Blend)." ABC Laboratories, Inc., Columbia, MO. Sponsor: American Chemistry Council, Arlington, VA
Other (source) Last changed	 1/31/06

2.2 ENVIRONMENTAL EXPOSURE AND FATE

2.2.2 Direct Photodegradation

Test Substance:	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	Other: Technical discussion
GLP	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Test Substance: **[components]**	Polyethylbenzene Bottoms (PEB, CAS RN 68987-42-8) is a co-product of ethylbenzene manufacture and a Class II complex mixture. It consists of various isomers of the following principal components. • Diphenylethanes • Diphenylmethanes • Triethylbenzenes • Diphenylpropanes
Light Source:	Not Applicable
Light Spectrum: • Wave length value (upper/lower)	Not Applicable
Relative Intensity:	Not Applicable
Test Substance Spectrum:	Not Applicable
Test Conditions: • Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol	Not Applicable
Direct Photolysis: • Results: half-life, % degradation, quantum yield	Not Applicable
Indirect Photolysis: • Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life	Not Applicable
Degradation Products: • Note: Identification, concentration	Not Applicable

<table>
<tr><td>Conclusion:</td><td>
<u>Technical Summary of Direct Photolysis</u>

Direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). If the absorbed energy is high enough, the resultant excited state of the chemical may transform to a different structure. A prerequisite for direct photodegradation is the ability of one or more bonds within a chemical to absorb ultraviolet (UV)/visible light in the 290 nm to 750 nm range. Light wavelengths longer than 750 nm do not contain sufficient energy to break chemical bonds, while wavelengths below 290 nm are shielded from the earth by the stratospheric ozone layer (Harris, 1982).

The majority of the constituents identified in PEB consist of various isomers of alkylbenzene and diphenyl structures. Harris (1982) notes that single ring aromatics do not absorb sufficient light energy above 290 nm to cause photolysis. Therefore, those types of constituents are not subject to photolysis. Similarly, diphenyl structures tend not to display absorbance maxima within the 290 – 750 nm range.

Characteristic absorbance maximum (λ_{max}) and molar extinction coefficients (ε) for three compounds, which were identified as components in PEB are shown below. Other constituents in PEB would have absorbance maxima and extinction coefficients in the range of those chemical.

<table>
<tr><th></th><th colspan="2"><u>λ below 290 nm</u></th><th colspan="2"><u>λ above 290 nm</u></th></tr>
<tr><th><u>Hydrocarbon</u></th><th>λ_{max}</th><th>ε</th><th>λ_{max}</th><th>ε</th></tr>
<tr><td>Cyclohexylbenzene</td><td>260</td><td>200</td><td>--</td><td>--</td></tr>
<tr><td>Diphenylmethane</td><td>260</td><td>470</td><td>--</td><td>--</td></tr>
<tr><td>1,2-diphenylethane</td><td>214</td><td>13,300</td><td>295</td><td>3000</td></tr>
</table>
Data from NIST Chemistry WebBook (http://webbook.nist.gov/chemistry)

Overall, this category of substances will not demonstrate a significant extent of degradation resulting from direct photolysis.
</td></tr>
<tr><td>Reliability:</td><td>1. Reliable without restrictions. The technical summary presented herein was based on a well-regarded scientific handbook and reference database.</td></tr>
<tr><td>Reference:</td><td>National Institute of Standards and Technology (NIST). 2003. NIST Standard Reference Database Number 69 – March 2003 Release. NIST Chemistry WebBook. http://webbook.nist.gov/chemistry

Harris, J.C. 1982. Rate of Aqueous Photolysis, Chapter 8 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.</td></tr>
<tr><td>Other (source):
Last changed</td><td>1/31/06</td></tr>
</table>

2.2.2 Indirect Photodegradation

Test Substance:	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	Calculated values using AOPWIN version 1.90, a subroutine of the computer program EPIWIN version 3.12 (U.S. EPA 2000) AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically-produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.
GLP	Not Applicable
Year (study performed):	Not Applicable
Test Substance: **[components]**	Polyethylbenzene Bottoms (PEB, CAS RN 68987-42-8) is a co-product of ethylbenzene manufacture and a Class II complex mixture. It consists of various isomers of the following principal components. • Diphenylethanes • Diphenylmethanes • Triethylbenzenes • Diphenylpropanes
Type (air, soil, water, other):	Not Applicable
Light Source:	Sunlight
Light Spectrum: • Wave length value (upper/lower)	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not Applicable
Test Conditions: • Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol	Atmospheric oxidation potential is an indirect photodegradation process that is based on the structure-activity relationship (SAR) developed by R. Atkinson (1988, 1989). The SAR assumes the following conditions: Temperature: 25°C Sensitizer: OH- radical Concentration of Sensitizer: $1.5E^{6}$ OH- radicals/cm^{3}
Direct Photolysis: • Results: half-life, % degradation, quantum yield	Not Applicable

Indirect Photolysis: • Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life	Calculated atmospheric oxidation potential (AOP) data for representative constituents of PEB are listed below. The data identify a potential AOP range for substances represented by the listed constituents. PEB does not have a specific atmospheric half-life; rather, actual half-life ranges for substances in this stream will vary dependent on their constituent composition. The compounds selected to represent the AOP range for PEB were selected on the basis of compositional analysis of a composite blend of streams from various suppliers. The following are AOP values calculated by the EPIWIN program: **Calculated OH- Rate Constant** **Substance Constituent** — **half-life (day)** — **(cm^3/molecule-sec)** Diethylbenzene — 1.3 — 8.1×10^{-12} 1,3,5-triethylbenzene — 0.32 — 1.4×10^{-11} 1,2,4-triethylbenzene — 0.60 — 3.3×10^{-11} Cyclohexylbenzene — 0.73 — 1.8×10^{-11} Diphenylmethane — 1.0 — 1.1×10^{-11} 1,1'-diphenylethane — 0.94 — 1.1×10^{-11} 1,2-diphenylethane (bibenzyl) — 0.89 — 1.2×10^{-11} 1,1'-diphenylpropane — 0.83 — 1.3×10^{-11}
Degradation Products: • Note: Identification, concentration	Unknown
Conclusion:	Atmospheric oxidation reactions from hydroxyl radical attack can significantly contribute to the degradation of constituent hydrocarbons in PEB. Constituent hydrocarbons have sufficiently high vapor pressures, indicating that such compounds will partition to air where oxidation reactions occur. Results from EQC Level 1 modeling of constituent hydrocarbons to assess environmental distribution support this evaluation. Based on calculated atmospheric oxidation potential values, hydrocarbons making up PEB have an atmospheric half-life range of approximately 0.3 to 1.3 days. These data suggest that the hydrocarbon constituents of this substance will degrade rapidly and not persist in the atmosphere.
Reliability:	**2.** Reliable with restrictions. Rate constants and half-lives presented in this robust summary were estimated using the AOPWIN program contained in the EPIWIN© model. They represent a potential range of atmospheric oxidation potentials based on constituent molecules in PEB.
References:	Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., New York, NY, USA. U.S. EPA. 2000. Estimations Programs Interface for Windows (EPIWIN©). U.S. Environmental Protection Agency, Washington, DC.
Other (source): Last changed	1/31/06

2.2.3 Stability in Water

Test Substance:	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	Other: Technical discussion
Type (test type):	Not Applicable
GLP	Not Applicable
Year (study performed):	Not Applicable
Analytical Monitoring:	Not Applicable
Test Conditions: • Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol	Not Applicable
Results: **Units/Value:** • Note: Analytical method, observations, half-lives by pH, degradation products	Not Applicable
Test Substance: **[components]**	Polyethylbenzene Bottoms (PEB, CAS RN 68987-42-8) is a co-product of ethylbenzene manufacture and a Class II complex mixture. It consists of various isomers of the following principal components. • Diphenylethanes • Diphenylmethanes • Triethylbenzenes • Diphenylpropanes
Conclusion:	**Technical Summary** Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Harris, 1982; Neely, 1985) . This reaction is referred to as nucleophilic substitution, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because carbon atoms lacks sufficient electronegativity to serve as a good leaving group (i.e., carbon-carbon bonds are too stable to be cleaved by nucleophilic substitution). Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Harris, 1982; Neely, 1985). The constituent compounds in PEB are hydrocarbons that contain only carbon and hydrogen. Thus, the PEB stream is not subject to hydrolysis,

	and this fate process will not contribute to the degradative loss of chemical constituents in this Class II complex mixture.
Reliability:	2. Reliable with restrictions. The technical summary presented herein was based on well-regarded scientific references.
Reference:	Harris, J.C. 1982. "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA Neely, W. B. 1985. “Hydrolysis”, Chapter 7 in: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I. 173. CRC Press, Boca Raton, FL, USA.
Other (source): Last changed	1/31/06

2.2.4 Transport Between Environmental Compartments

Test Substance:	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	Calculated according to EQC Level 1 Model Version 2.02 (Trent University, 2003)
Type (test type):	Not Applicable
GLP:	Not Applicable
Year (study performed):	Not Applicable
Estimation Temperature:	25°C
Test Conditions: • Note: Concentration prep., vessel type, replication, test conditions**.**	The EQC model uses chemical-physical properties to quantify a chemical's behavior in an evaluative environment. It calculates the distribution of a fixed quantity of conserved (i.e., non-reacting) chemical, in a closed environment at equilibrium, with no degrading reactions, no advective processes, and no inter-media transport processes (e.g., no wet deposition, or sedimentation). The medium receiving the emission is unimportant because the chemical is assumed to become instantaneously distributed. Physicochemical input values (molecular weight, water solubility, vapor pressure, partition coefficient, and melting point) for the EQC model were obtained from EPIWIN (U.S. EPA, 2000) database. Measured values for input parameters were used when available; otherwise, modeled values were employed.
Results: **Units/Value:** • Note: Deviations from protocol or guideline, analytical method.	Calculated partitioning data for representative constituents of PEB are listed below. The range of distribution data for constituent chemicals in each of the compartments can be used as an estimate of the partitioning behavior for such streams.

Substance	**Calculated Percent Distribution**					
Constituent	**Air**	**Water**	**Soil**	**Sed.**	**Sus.Sed**	**Biota**
Diethylbenzene	79.2	0.6	19.8	0.4	<0.1	<0.1
Cyclohexylbenzene	35.3	1.1	62.2	1.4	<0.1	<0.1
1,3,5-triethylbenzene	99.8	<0.1	0.2	<0.1	<0.1	<0.1
1,2,4-triethylbenzene	75.6	0.2	23.7	0.5	<0.1	<0.1
Diphenylmethane	16.3	6.2	75.8	1.7	<0.1	<0.1
1.1'-diphenylethane	28.5	5.2	64.9	1.4	<0.1	<0.1
1,2-diphenylethane	12.7	1.5	83.8	1.9	<0.1	<0.1
1,1'-diphenylpropane	11.9	2.2	84	1.9	<0.1	<0.1

Test Substance:	Polyethylbenzene Bottoms (PEB, CAS RN68987-42-8) is a co-product of ethylbenzene manufacture and a Class II complex mixture. It consists of various isomers of the following principal components. • Diphenylethanes • Diphenylmethanes

	• Triethylbenzenes • Diphenylpropanes
Conclusion:	The partitioning data represent a potential distribution range for constituent hydrocarbon chemicals in PEB. These hydrocarbons were calculated to partition either to air or soil depending in large part on the number of ring constituents in the molecule. With the exception of cyclohexylbenzene, alkylbenzene constituents were shown to partition primarily to air and secondarily to soil. Cyclohexylbenzene and biphenyl compounds partitioned primarily to soil and secondarily to air. A small percentage of all compounds (<0.1 to 6.2%) partitions to water or sediment (<2%). The input data used to run the EQC Level I model preferentially used measured data from the EPIWIN database and estimated values calculated by the EPIWIN program based on chemical structure when measured data were not available.
Reliability:	**2.** Reliable with restrictions. The environmental distribution data presented in this robust summary were estimated using the EQC model developed by Trent University. They represent the potential environmental distribution of the test substance based on constituent molecules in PEB.
Reference:	Trent University. 2003. EQC Fugacity-Based EQC-Equilibrium Criterion Model. Canadian Environmental Modeling Centre, Trent University, Peterborough, Ontario (http://www.trentu.ca/cemc/). U.S. EPA. 2000. Estimations Programs Interface for Windows (EPIWIN). U.S. Environmental Protection Agency, Washington, DC.
Other (source): Last changed	 1/31/06

2.2.5 Biodegradation

Test Substance:	Polytheylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	OECD Method 301D (1992)
Type (test type):	Aerobic biodegradability (Ready)
GLP:	Yes
Year (study performed):	2005
Inoculum:	Secondary effluent from a wastewater treatment plant
Test Conditions:	Secondary effluent from the Columbia Wastewater Treatment Plant (Columbia, Missouri) was collected and brought into the laboratory. Approximately 0.5 L of the secondary effluent was filtered through glass wool, with the first 200 mL of filtrate being discarded. Seventy-five milliliters of the filtrate was reserved and added to 14 L of nutrient medium. The inoculated mineral salts medium was aerated at 20 °C for approximately 4 days before use. Bulk testing solutions were prepared in 4-L Nalgene carboys by adding 3,992mL of inoculated medium to each of three carboys followed by either 8mL of sodium benzoate stock solution (reference substance treatment at 2mg/L nominal concentration), 8 mg of test sustance plus 8 mL of reagent water(PEB Blend treatment at 2 mg/L nominal concentration), or 8 mL of reagent water (control). The bulk test solutions were stirred for at least 30 min. Each testing solution was transferred to 10 clean BOD bottles by draining from the carboys. All BOD bottles were sealed without any headspace using glass stoppers. Duplicate BOD bottles were randomly designated for sampling and Day-0 bottles were removed for dissolved oxygen analyses. The remaining bottles were incubated in the dark on an orbital shaker in an environmental chamber set at 20 °C. Dissolved oxygen measurements were measured using a dissolved oxygen meter and probe on Days 0, 8, 14, 21, and 28. Solution pH was measured on Day 0 and 28. Bacterial plate counts were performed on the inoculated mineral salts at initiation and one of the duplicate BOD bottles for each treatment at Day 28. The mineral salts solution at the beginning of the test was 1.4×10^5 colony forming units (CFU)/mL, while Day 28 solutions of the control, reference substance, and the test substance contained 1.8×10^4, 7.5×10^3, and 6.5×10^3 CFU/mL, respectively, and indicated that the microbial inoculum remained viable through the end of the test in each experimental group. Biochemical oxygen demand (BOD) was calculated from the measured oxygen concentrations taken in the BOD bottles using the following equation: $BOD\ (mg\ O_2/mg\ substance) = (DO_T - DO_B)/C_T$, where DO_T = dissolved oxygen uptake for the test or reference substance (mg O_2/L), DO_B = dissolved oxygen uptake in the blank (mg O_2/L), and C_T = test concentration of the test or reference substance

	(mg/L). Biodegradation of the test and reference substances was calculated as a percentage of the theoretical oxygen demand (ThOD) using the following equation: % Biodegradation = (BOD/ThOD) x 100 The ThOD was determined to be 1.67 mg O_2/mg for sodium benzoate and 3.09 mg O_2/mg for PEB Blend using elemental analyses and the equation for ThOD without nitrification in the OECD guideline.
Results: Kinetic for each time period: Breakdown products:	PEB Blend: 7.1 % biodegradation after 28 days Sodium Benzoate: 88.6 % biodegradation after 28 days Percent Biodegradation Day — PEB Blend — Sodium Benzoate 8 — 0 — 82.9 14 — 3.7 — 83.8 21 — 1.8 — 83.5 28 — 7.1 — 88.6 N/A There were no deviations from the protocol or guideline.
Conclusions: (Laboratory Contractor)	The test substance showed a maximum of 7.1% biodegradaton throughout the 28-day test indicating that PEB Blend is not readily biodegradable.
Reliability:	**1**. Reliable without restrictions.
Reference:	Serak, Kelda. 2005. Determination of the Ready Biodegradability of Polyethylbenzene Bottoms Stream Blend (PEB Blend) Using the Closed Bottle Test Method. ABC Laboratories, Inc., Columbia, MO. Sponsor: American Chemistry Council, Arlington, VA
Other (source) Last changed	 4/1/06

3.1 HAZARDS TO THE ENVIRONMENT: AQUATIC EFFECTS

3.1.1 Invertebrate Acute Toxicity

Test Substance	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/guideline	OECD Guideline 202, Part 1 (1992)
Type (test type)	Static-renewal, water accommodated fraction
GLP	yes
Year (study performed)	2005
Species	*Daphnia magna*
Analytical Monitoring	yes
Exposure Period	48 hours
Statistical Methods:	EC50 by the Trimmed Spearman-Karber Method
Test Conditions: Note: concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, supplier of organisms, age, size, loading	The PEB sample was a blend of equal volumes of six PEB samples from different suppliers.Groups of *Daphnia magna* were exposed to a negative control, a solvent control (0.05 mL acetone/L) and five concentrations of the test substance and assessed for immobilization for 48 hours. Exposure solutions were prepared as water accommodated fractions (WAFs) of Polyethylbenze Bottoms (PEB) blend, and exposure solutions were renewed at 24 hours using fresh WAFs. The experimental treatments included control, solvent control, and five PEB loading rates of 65, 130, 250, 500, and 1000 μg/L. WAFs were prepared by adding appropriate volumes from five stock solutions of the test substance to 2.0 L of dilution water in each of five 2.0-L glass aspirator bottles. Each bottle was sealed with parafilm and stirred with a teflon stir bar for approximately 2 hours. Stirring speed was adjusted to create a slight vortex in each bottle (<25% of the solution depth). Once the stirring period ended, the liquid phases in the bottles were allowed to separate for approximately 30 min. Control (dilution water) and solvent control (0.05 mL acetone/L) solutions were treated in the same manner. From each aspirator bottle, solution was drained from the bottom outlet into four replicate 8-oz (237-mL) glass jars, which served as test vessels. Vessels were completely filled and sealed with a glass plate to eliminate all headspace. Remaining solution from each aspirator bottle was used for water quality measurements and analysis for the test substance. Dilution water used in testing and culturing daphnids was aged laboratory freshwater prepared by blending naturally hard well water with well water that was de-mineralized by reverse osmosis. The waters were blended to yield a total hardness of 130 to 160 mg/L as $CaCO_3$ and biologically aged. First-instar neonates, less than 24 hours old were used to initiate the test. Neonate daphnids originated from cultures maintained in the testing laboratory, where adults were fed at least once a day a suspension of the alga, *Pseudokirchneriella subcapitata*, supplemented by a prepared artificial invertebrate food. Daphnids used in testing were not fed. Adults that produced the young were approximately 18 days old and showed no signs of stress or physical damage.

Five daphnids were randomly assigned and carefully transferred to each of four replicate test vessels, giving a total of 20 daphnids for each experimental group. Vessels were place in a 20 ± 1°C temperature-controlled waterbath. Lighting was provide by fluorescent bulbs at an intensity of 502 lux at the level of the test vessels. A photoperiod of 16-hour light and 8-hour dark with a 30 min dusk/dawn transition period was used during the test. Numbers of immobilized daphnids were recorded at 24 and 48 hours.

The concentrations of PEB in the WAF solutions were measured in samples collected at 0 hour (fresh solutions), 24 hours (fresh and old solutions), and 48 hours (old solutions). Analyses were done using gas chromatography with a flame ionization detector. Responses of standards and samples were calculated as the sum of the responses from six marker peaks within the PEB chromatogram.

Temperature measurements of the exposure solutions during the test ranged from 19.0 °C to 19.8 °C, dissolved oxygen ranged from 8.0 mg/L to 8.7 mg/L, and the pH in all solutions was 8.3 for the duration of testing. Hardness, alkalinity, and specific conductance of the dilution water at test initiation were 412 mg/L as $CaCO_3$, 156 mg/L as $CaCO_3$, and 347 µS, respectively. Measured concentrations of PEB in WAF solutions were:

Nominal Loading Rate µg/L	0-hr fresh	24-hr old	24-hr fresh	48-hr old	mean	% nominal
Control	<MQL	< MQL	< MQL	< MQL	< MQL	--
Solv. Control	< MQL	< MQL	< MQL	< MQL	< MQL	--
65	60.6	60.4	61.9	61.1	61	94
130	120	110	131	105	117	90
250	237	233	234	122	207	83
500	464	452	466	468	463	93
1000	918	868	977	842	901	90

Minimal Quantifiable Limits [MQL] = 41.6 µg/L

Results

Units/Value:

Note: Deviations from protocol or guidelines, analytical method, biological observations, control survival

24-hour EC50 = >1000 µg/L, based on nominal WAF loading rates

48-hour EC50 = 340 µg/L, based on nominal WAF loading rates.

95% confidence limits = 310 µg/L and 310 µg/L.

48-hour No-Observed-Effect Concentration = 130 µg/L

The slope of the dose-response line at 48-hours was 9.7.

The following dose response at 48 hours was obtained in the test.

Nominal Loading Rate, µg/L	48-hour % Immobilized
Control	0
Solvent control	0
65	0
130	0
250	10
500	95
1000	95

There were no deviations from the protocol or guideline.

Conclusions

24-hour EC50 = >1000 µg/L based on nominal WAF loading rates

(Laboratory contractor)	48-hour EC50 = 340 μg/L based on nominal WAF loading rates. 48-hour NOEC = 130 μg/L The 48-hour dose-response slope = 9.7
Reliability	**1.** Reliable without restrictions
Reference	Analytical Bio-Chemistry Laboratories (ABC). 2005. Acute toxicity of polyethylbenzene bottoms stream blend (PEB) to the water flea, Daphnia magna, determined under static-renewal test conditions. ABC Study No. 49029, ABC Laboratories, Columbia, MO. Sponsor: American Chemistry Council, Arlington, VA
Other Last changed	 1/31/06

3.1.2 Fish Acute Toxicity

Test Substance:	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/guideline:	OECD Guideline 203 (1992)
Type (test type):	Static-renewal, water accommodated fraction
GLP:	yes
Year (study performed):	2006
Species:	fathead minnow (*Pimephales promelas*)
Analytical Monitoring:	yes
Exposure Period:	96 hours
Statistical Methods:	LC50 by the probit method and the untrimmed Spearman-Karber method.
Test Conditions: Note: concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, supplier of organisms, age, size, loading	The PEB sample was a blend of equal volumes of six PEB samples from different suppliers. Groups of fathead minnows were exposed to a negative control, a solvent control (0.05 mL acetone/L), and five concentrations of the test substance for 96 hours. Fish were assessed for mortality and abnormal behavior effects each day. Exposure solutions were prepared as water accommodated fractions (WAFs) of Polyethylbenzene Bottoms (PEB) blend, and exposure solutions were renewed every 24 hours using fresh WAFs. The experimental treatment included control, solvent control, and five PEB loading rates of 3.3, 6.5, 13, 25 and 50 mg/L. Dilution water was laboratory freshwater prepared by blending naturally hard well water with well water that was demineralized by reverse osmosis WAFs were prepared by direct addition of 0.0312, 0.0614, 0.123, 0.236, and 0.473 mL volumes of PEB (density = 0.9526 g/mL) to respective 9.5-L glass carboys, each containing 9 L of dilution water. The solvent control carboy and the five carboys containing PEB received 0.450 mL acetone. Each carboy was sealed with parafilm and stirred with a teflon stir bar for approximately 2 hours. Stirring speed was adjusted to create a slight vortex in each bottle (<25% of the solution depth). Once the stirring period ended, liquid phases in the carboys were allowed to separate for approximately 30 min. Control (dilution water) and solvent control (0.05 mL acetone/L) solutions were treated in the same manner. From each carboy, solution was siphoned into two replicate 3.8-L glass jars, which served as test chambers. The test jars were completely filled such that each chamber held approximately 3.8 L and contained no headspace when jars were sealed with a glass plate. This procedure of test solution preparation was repeated on days 1, 2, and 3. A film was observed on the surface of all test solutions that appeared to increase with increasing concentration. . Fish used in the test originated from established in-house cultures maintained by the testing laboratory. Fish were cultured in the same water as used in testing and at approximately the same temperature. Fish were fed newly hatched brine shrimp (*Artemia* sp.) and a commercial fish food two times a day while in culture. Fish were not fed approximately 48 hours prior to testing or during the test. There were

no mortalities in the culture the nine days prior to initiation of the definitive test. Fish selected for the test were approximately two months old and ranged from 22 to 26 mm in total length (mean and standard deviation (SD) = 24 mm ± 1.5mm) and 0.076 to 0.151 g blotted wet weight (mean and SD = 0.118 ± 0.0267 g). The loading rate was 0.155 g fish/L of test solution.

Once the test chambers were filled with test solution, fish were distributed one at a time until each test chamber contained its complement of five fish, giving 10 fish per each experimental group. Test chambers were sealed with a glass plate and were not opened except when fish were transferred to newly-prepared WAF solutions at 24, 48, and 72 hours. Test chambers were placed in a temperature-controlled waterbath set to maintain a temperature of 23 ± 1°C. Fluorescent lighting was maintained on a 16-hour daylight photoperiod with 30-min simulated dawn and dusk periods. Light intensity during the test was 763 lux.

Temperature, dissolved oxygen, and pH were measured in all fresh solutions at 0, 24, 48, and 72 hours, and in all old solutions at 24, 48, 72, and 96 hours. Measurements for dissolved PEB in the test solutions were made on fresh solutions collected at 0 and 72 hours, and on old solutions collected at 24 and 96 hours. Samples were analyzed by gas chromatography (GC) using flame ionization detection (FID). Concentrations of dissolved PEB were calculated from a standard curve as the sum of the responses from six marker peaks within the PEB chromatogram.

Temperature measurements of the exposure solutions during the test ranged from 22.7° C to 23.7° C, dissolved oxygen ranged from 7.9 mg/L to 8.4 mg/L in the new solutions and from 6.2 to 7.2 mg/L in the old solutions. The pH of the fresh solutions ranged from 7.62 to 7.98 and from 7.56 to 7.80 in the old solutions. The dilution water at test initiation had a total hardness of 140 mg/L as $CaCO_3$, total alkalinity of 150 mg/L as $CaCO_3$, and conductivity of 357 µS.

Measured concentrations of PEB in the WAF solutions were:

Nominal Loading Rate, mg/L	0-hr fresh	24-hr old	72-hr fresh	96-h old	mean	% nominal
Control	<MQL	<MQL	<MQL	<MQL		
Solv. Control	<MQL	<MQL	<MQL	<MQL		
3.3	0.795	0.669	0.876	0.792	0.783	24
6.5	0.943	0.840	1.22	1.13	1.03	16
13	1.14	0.945	1.97	1.91	1.49	11
25	1.50	1.27	2.27	2.22	1.82	7
50	2.82	2.28	NS	NS	2.55	5

Minimum Quantifiable Limit (MQL) = 0.208 mg/L

Results

Units/Value:

Note: Deviations from protocol or guidelines, analytical method, biological observations, control survival

96-hour LC50 = 1.65 mg/L (95% C.L. = 1.43 and 1.87 mg/L), based on mean measured PEB concentrations.

96-hour NOEC = 1.03 mg/L, based on mean measured PEB concentrations.

96-hour dose-response slope = 14

Nominal Loading Rate, mg/L	Mean Measured Conc, mg/L	Mean 96-hour % Mortality
Control	<MQL	0
Solv. Control	<MQL	0
3.3	0.783	0
6.5	1.03	0
13	1.49	30

	25 1.82 70 50 2.55 100 There were no protocol or guideline deviations that adversely affected the study.
Conclusions (Laboratory contractor)	96-hour LC50 = 1.65 mg/L based on mean measured concentrations 96-hour NOEC = 1.03 mg/L based on mean measured concentrations The 96-hour dose-response slope = 14
Data Quality Reliabilities	1. Reliable without restrictions
Reference	Analytical Bio-Chemistry Laboratories (ABC). 2006. Acute toxicity of polyethylbenzene bottoms stream blend (PEB Blend) to the fathead minnow, *Pimephales promelas*, determined under static-renewal test conditions. ABC study No. 49028, ABC Laboratories, Columbia, Missouri. Sponsor: American Chemistry Council, Arlington, VA.
Other Last changed	6/19/06

3.1.3 Toxicity to Aquatic Plants (e.g., algae)

Test Substance:	Polytheylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	OECD Method 201
Type (test type):	static, water accommodated fractions in sealed vessels
GLP:	yes
Year (study performed):	2005
Species/strain no. and source:	*Pseudokirchneriella subcapitata* obtained from University of Texas - Austin
Element Basis:	area under the growth curve, growth rate
Exposure Period:	72 hours
Analytical Monitoring:	yes
Statistical Methods:	EC values determined using a logistic model; NOEC values determined using one-way ANOVA with Dunnett's test
Test Conditions: Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organism supplier, age, size, loading.	The PEB sample was a blend of equal volumes of six PEB samples from different suppliers. Exposure solutions of PEB were prepared as water accommodated fractions (WAF) in freshwater algal nutrient medium. The medium was prepared according to guideline procedures and supplemented with $NaHCO_3$ (500 mg/L) by adding quantities of reagent grade salts to purified and sterilized water. After adding the salts, the medium was pH-adjusted to 7.5 ± 0.1 using 0.1 N HCl. WAF solutions were prepared by adding 0.10-mL volumes of PEB Blend standards made in acetone to 2.0 L of medium in a 2.0-L glass aspirator bottle. Each aspirator bottle was sealed and stirred for approximately 1.8 hours. Stirring was adjusted to create a vortex of no greater than 25% of the height of the solution in the bottle. After stirring, the solutions were allowed to settle for 40 minutes. The aqueous phase was drawn from the bottom of each aspirator bottle into nine replicate test flasks. WAF solutions were created in this manner for PEB Blend loading rates of 65, 130, 250, 500, and 1000 µg/L. A negative control and a vehicle control with acetone at 0.05mL/L were prepared in a similar fashion. The 130mg/L treatment contained an additional replicate that served as an abiotic control group. This replicate was not inoculated with algae. Replicate flasks consisted of 125-mL Erlenmeyer flasks with Teflon®-lined screw caps. When completely filled and sealed with no headspace, flasks held approximately 147 mL of test solution. Replicates were filled and sealed in this manner to minimize potential loss of volatile components in the test substance. The freshwater alga, *Pseudokirchneriella subcapitata*, was maintained in the laboratory in liquid cultures. The origin of the culture was the Department of Botany, Culture Collection of Algae, University of Texas at Austin. New cultures were periodically cloned from the existing culture derived from the parent stock. The culture used in this test was seven days old at test initiation. The test commenced when the flasks were filled, inoculated with algae to a starting density of approximately 1.0×10^4 cells/mL, sealed, and randomly placed on a rotary shaker set a approximately 100 rpm. Flasks were incubated at 24 ± 2°C for 72 hours under continuous lighting. Lighting was

	produced by cool-white fluorescent bulbs at an intensity of 8,600 ± 10% lux. Temperature and light intensity were monitored throughout the study. Cell densities were determined using a light microscope and a haemacytometer at 24, 48, and 72 hours. At each counting period, three replicate flasks were destructively sampled and counts were made of the cell densities in each replicate flask. At the beginning of the test, measurements of pH were made in samples taken from the aspirator bottle of each treatment. At the end of the test, pH of the solution in the first replicate of each treatment was measured. The temperature of the testing area was measured continuously during the test. The pH of the test solutions ranged from 7.9 to 8.0 at test initiation and from 8.0 to 9.4 at 72 hours. Temperature of the test solutions ranged from 22.6°C to 23.0°C when measured at 0 and 72 hours. The continuous temperature recording of the testing area ranged from 23.7°C to 24.4°C. The area under the curve, and growth rate were taken as indices of algal growth and were calculated for each treatment using cell densities determined at 24, 48, and 72 hours. **Area Under the Growth Curve (AUGC):** $A = (N_1 – N_0/2) \times t_1 + (((N_1+N_2 - 2N_0)/2) \times (t_2 – t_1))) +…+(((N_{n-1} + N_n – 2N_0)/2) \times (t_n – t_{n-1}))$ A= area under the growth curve N_0 = Nominal number of cells at t_0 N_1 = Mean cell density at t_1 N_2 = Mean cell density at t_2 N_n = Mean cell density at t_n t_1 = time of first measurement (hours from start) t_2 = time of first measurement (hours from start) t_n = time of nth measurement (hours from start) **Growth Rate:** $\mu = ((\ln N_n – \ln N_0)/(t_n – t_0))$ μ = average specific growth rate N_0 = Nominal cell density at t_0 N_n = Measured dell density at t_n t_0 = Time of beginning of test (hours) t_n = Time after beginning of test (hours) The response of the negative and vehicle control groups was assessed to determine whether or not they could be pooled by comparing the 72-hour means for the area under the growth curve and growth rate. Tests for normality and homogeneity of variance were performed along with a t-test between the two control groups. The analyses showed a statistical difference between the control groups for biomass and growth rate; therefore, the vehicle control response was used for the calculation of inhibition values for the treatment group's responses. **Calculation of Inhibition:** Percentage inhibition of growth (I_A) and growth rate (I_u) were calculated by the following equation: Inhibition, % = (vehicle control mean – treatment mean) / vehicle control mean x 100 Concentrations of PEB Blend in the WAF solutions were measured by gas

	chromatography in samples from each treatment level at the beginning and end of the test. Measurements were based on a validated method that summed the responses from six marker peaks within the PEB Blend chromatogram. Concentrations were determined directly from a standard curve. Measured concentrations of PEB in the WAF solutions were: Nominal Loading Rate, µg/L / 0-hr fresh / 72-hr old / mean / % nominal Control / <MQL / <MQL Solvent Control / <MQL / <MQL 65 / 50.9 / 37.8 / 44.4 / 68 130 / 113 / 78.7 / 95.9 / 74 250 / 227 / 157 / 192 / 77 500 / 453 / 349 / 401 / 80 1000 / 754 / 627 / 691 / 69 Minimum Quantifiable Limit (MQL) = 41.6 µg/L
Results: Nominal Loading Rate Conc., µg/L	0 (control), 0 (vehicle control), 65, 130, 250, 500, and 1000 µg/L
Mean Measured Conc., µg/L	0 (control), 0 (vehicle control), 44.4, 95.9, 192, 401, and 691 µg/L
Element Values	72-h E_bC50 = 320 µg/L (95% CL = 310 and 330 µg/L) (nominal loading rate) 72-h E_rC50 = 640 µg/L (95% CL = 610 and 680 µg/L) (nominal loading rate) 72-h NOEC = 130 µg/L (nominal loading rate) 72-h E_bC50 = 251 µg/L (95% CL = 241 and 261 µg/L) (mean measured concentration) 72-h E_rC50 = 485 µg/L (95% CL = 463 and 507 µg/L) (mean measured concentration) 72-h NOEC = 95.9 µg/L (mean measured concentration) Negative and vehicle control responses over the 72-h period exceeded the minimum acceptable increase in cell density as specified in the guideline.
Conclusion: (Laboratory Contractor)	The 72-hour NOEC was the nominal loading rate of 130 µg/L or the mean measured concentration of 95.9 µg/L, based on a lack of statistically significant reduction of biomass and growth rate at or below this test substance treatment. Based on biomass, the 72-hour E_bC_{50} was the nominal loading rate of 320 µg/L or the mean measured concentration of 251 µg/L. Based on growth rate, the 72-hour E_rC_{50} was the nominal loading rate of 640 µg/L or the mean measured concentration of 485 µg/L.
Reliability:	**1**. Reliable without restrictions.
Reference:	Hicks, Stephen L. 2006. Toxicity of a Polyethylbenzene Bottoms Stream Blend (PEB Blend) to the Unicellular Green Alga, *Psudokirchneriella subcapitata*. ABC Laboratories, Inc., Columbia, MO. Sponsor: American Chemistry Council, Arlington, VA
Other (source) Last changed	8/14/06

4.0 HUMAN HEALTH HAZARDS

4.1.1 Acute Oral Toxicity

Test Substance:	Polytheylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	FIFRA/TSCA guidelines
Type (test type):	LD_{50}
GLP:	Not stated
Year (study performed):	1985
Species/strain:	Rats - Fisher 344
Sex:	Male and female
No. of animals/sex/dose:	5
Route of Administration:	Oral gavage
Vehicle:	None
Test Conditions:	The test material is a single PEB sample from Gulf Oil Co. At the start of the experiment, animals were 65 days old with a weight ranging from 113 to 166 grams. During the study, room temperature averaged 72.8^{o}F, and relative humidity averaged 55%. Each animal was observed at 1 hr and 4 hr after administration of the test substance and at least once daily for 14 days post dosing
Results:	LD_{50} > 5.0g/kg No mortality was observed during the study. Soft feces were observed at the 4-hour observation and on Days 2 and 3. Anogenital soiling was noted at the 4-hour observation and on Days 2, 3, 6, and 8. Brown material around the nose and mouth was seen on some animals on Days 2 and 3. All animals were normal on Days 2 and 3. All animals were normal for all clinical observation intervals from Day 9 until study termination. No adverse effects on body weights were observed throughout the study. Gross necropsies of the animals were performed and the observed tissues were within normal limits for the species.
Conclusion: (Laboratory Contractor)	Based on the lack of mortality at 5.0 g/kg, PEB was assigned a descriptive classification for acute oral exposure of "practically non-toxic".
Reliability:	**1b**. Reliable without restrictions, comparable to a current guideline study.
Reference:	Gulf Life Science Center. 1985. Acute Oral Toxicity Study in Rats of Polyethylene Bottoms. Project No. 84-2133
Other (source) Last changed	 10/20/03

4.1.1 Acute Dermal Toxicity

Test Substance:	Polytheylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	Not specified
Type (test type):	Five-day repeated dose
GLP:	Not stated
Year (study performed):	1985
Species/strain:	Rats - Fisher 344
Sex:	Male and female
No. of animals/sex/dose:	5
Route of Administration:	Dermal
Doses/concentration levels	0 [Vehicle Control], 1g/kg 50% PEB Bottoms; 2.0g/kg 100% PEB Bottoms
Vehicle:	Light paraffin oil [CAS # 8012-95-1
Test Conditions:	The test material is a single PEB sample from Gulf Oil Co. At the start of the experiment, animals were 70 days of age and weighed between 129.27g to 206.32g. During the study, animal rooms were maintained at an average ambient temperature of 73.6^0F and relative humidity of 55.5% Prior to treatment initiation, the backs of all animals were clipped free of hair. Each animal was fitted with an Elizabethan collar to prevent ingestion of test or control substances. The three dose groups consisted of: vehicle control (light paraffin oil) [Group I], diluted low-dose (50%) 1g/kg PEB Bottoms [Group II], high dose (100%) 2g/kg PEB Bottoms [Group III]. The appropriate doses or test control substance were applied topically to the prepared back of 5 test animals per group for a period of 6 hours. Treatment was performed once daily for a total of 5 doses. Animals were observed daily for clinical signs, mortality and moribundity. Dermal reactions were observed and scored twice on the initial dosing day and at the time of residual test substance removal. The Draize Scoring System for evaluating dermal reactions was used for scoring purposes. Body weights were recorded immediately prior to initial treatment and again at necropsy. All animals surviving to the scheduled study termination were sacrificed on Day 8 and gross necropsies on all animals were performed.
Results:	All animals survived to the termination of the study. No mortality occurred as a result of the 5-day repeated dermal application of Polyethylbenzene Bottoms to male and female rats at dose levels of 1.0 g/kg (Group II) and 2.0 g/kg (Group III). Statistical analyses of group mean body weights revealed weight losses among males and females at both the 1.0 and 2.0 g/kg dose levels that were significant at the 99% confidence level. A yellow brown discoloration of the test site was seen among all animals treated with the test substance. Dermal irritation was observed among animals in Groups II and III. Barely perceptible erythema was observed in the Group II (1.0 g/kg) animals. Erythema (ranging from very slight to well defined) and barely perceptible edema were seen among animals in Group III (2.0 g/kg).

	Focal thickening of the skin at the point of application of the test substance was observed in Group III (2.0 g/kg).
Conclusion: (Laboratory Contractor)	Dermal application at 1.0 or 2.0g/kg on five consecutive days to rats resulted in no mortality; body weights were decreased at both dose levels.
Reliability:	**2a**. Reliable with restrictions; acceptable, well-documented study report which meets basic scientific principles.
Reference:	Gulf Life Sciences Center. 1985. Five –Day repeated dose dermal toxicity study in rats of Polyethylbenzene Bottoms. Project No. 84-2137
Other (source) Last changed	 10/20/03

4.1.4 and 4.17 Repeated Dose Toxicity Study with Reproductive/Developmental Screening

Test Substance:	Polyethylbenzene Bottoms Stream (PEB Bottoms) is 100% of the complex mixture CAS RN. 68987-42-8. PEB Bottoms is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	OECD Guideline 422 (1996)
Type (test type):	28 day repeated dose oral toxicity study with neurobehavioral endpoints and reproductive/developmental screening
GLP:	Yes
Year (study performed):	2005
Species/Strain	Rats – Sprague Dawley
Route of Administration	Oral gavage
Duration of Test	Approximately 8 weeks
Doses/concentration levels	0, 20, 80, and 320 mg/kg/day
Sex	12 males and 12 females/group
Exposure period	Males 35-37 days; Females, max. 52 days [2 wks premating, 2 wks mating, gestation days (GD) 0-21 to lactation days (LD) 3-4].
Frequency of Treatment	Once/day, 7 days/week
Control group and Treatment	12 males, 12 females Corn oil, 5ml/kg/day, 7 days/wk
Statistical Methods:	2-tailed tests at 1 and 5% significance levels. Litter was experimental unit as appropriate. Data from non-gravid females excluded following mating period. Chi square was used for mating, fertility, conception and copulation indices. Parametric one-way analysis of variance (ANOVA) for body wt and wt gains [parents and offspring] food consumption, number of pups, live litter size at postnatal (PND) 0, unaccounted for sites, clinical pathology, absolute and relative organ wt, precoital intervals, Functional Observational Battery (FOB) data. If intergroup variances were seen, Dunnett's test used for comparisons between groups. Kruskal Wallis nonparametric ANOVA was used for percentage of males/litter at birth, postnatal survival, then Dunn's test was used for group comparisons. FOB parameters yielding scalar or descriptive data were analyzed by Fisher's exact test. Locomotor activity parameters were analyzed by repeated measure analysis of variance (RANOVA). Sequential linear trend tests were used for monotonic dose response relationships. Non-monotonic trends, evaluated whenever no significant linear trends were detected by treatment (TRT) and/or the TRT*TIME interaction was significant at the 0.01 level, were analyzed within the RANOVA pair-wise comparison package. Total count locomotor activity data were analyzed at BioSTAT Consultants, Inc., Portage, MI. Ambulatory counts were subjected to one-way ANOVA then Dunnett's if appropriate.

Test Conditions	The PEB Bottoms sample was a blend of equal volumes of six PEB Bottoms samples from different suppliers. Sprague Dawley rats (56 days of age) were received from Charles River Laboratories, Raleigh, NC and acclimated for 16 days. Twelve males (322.8 – 390.8g, 10 wks of age) and 12 females (201.5 – 258.8g, 10 wks of age) were assigned to each treatment group. PEB Bottoms in corn oil was administered in doses of 0, 20, 80 and 320mg/kg once daily by oral gavage, 7 days/wk. Males were treated from 14 days prior to mating to 1 day prior to sacrifice or on the day of sacrifice for males assessed for neurobehavioral parameters for a total of 37-39 days. Females were treated from 14 days prior to mating through gestation to lactation day (LD) 3 or 4 if assessed for neurobehavioral parameters for a total of 39 (non-mated females) to 52 doses. Animals were housed in individual stainless steel wire mesh cages until mating, then paired 1:1 in the male's home cage. Following copulation confirmed by vaginal plug or sperm in vaginal lavage sample, designated gestation day (GD) 0, females were transferred to plastic boxes with ground corncob bedding (Bed-O'Cobs® - analysis from manufacturer) as nesting material. Females remained housed in these boxes until sacrifice at LD 4. Food and water was available *ad libitum*. Room conditions were 22±3^{0}C average temperature, 50±20% humidity with a 12-hour light/dark cycle and 12 air changes/hr. Analysis: Dosing solutions were prepared weekly. Dosing solutions were evaluated for homogeneity, resuspension homogeneity, and stability prior to study initiation and samples were taken during the study to verify concentrations at each dose level for the first two weeks of administration and monthly thereafter. Four major peaks areas were identified for PEB Bottoms in corn oil by gas chromatographic analysis at retention times of 8.0, 9.6, 10.0 and 10.2 minutes. Concentrations were back calculated from results of regression analysis of the sum of these 4 major peaks. A Certificate of Analysis of the major components of PEB Bottoms was supplied with this study. Clinical Observations: All rats were observed twice daily for moribundity and mortality. Clinical observations were recorded daily. Once prior to study initiation and weekly thereafter, rats were observed outside the home cage for behavioral changes. Animals were observed at dosing and 1 hour after dosing for signs of overt toxicity. Body weights and Food consumption: Body wt data were recorded weekly for males and females until beginning of gestation. Thereafter female body weights were recorded at GD 0, 4, 7, 11, 14, 17, 20 and LD 1 and 4. Weights of non-pregnant females were recorded weekly. Food consumption was recorded over the same intervals except during mating. Parturition: Pregnant rats were observed twice daily for initiation and completion of parturition and signs of dystocia. On postnatal day 0 pups were sexed and examined for malformations, and the number of stillborn and live pups were recorded. Gestation length was calculated from the date at which parturition began. Neurobehavioral Parameters: FOB [Functional Observational Battery] observations were recorded for 6 rats/sex/group during week 5 (males) and on LD 4 (females) approximately 1 hour postdose. Testing was performed by the same technicians without knowledge of group assignment in a sound-attenuated room with a white noise generator set at 70±10dB. Observations included home cage and handling, open field, sensory (e.g. startle response, forelimb and hindlimb extension, air righting reflex, tail pinch), neuromuscular observations (e.g. hindlimb foot splay, fore and hindlimb grip strength, rotarod performance),

	and physiological observations (catalepsy, body wt, body temperature). Locomotor activity was recorded after completion of FOB using a photobeam activity system. Data were collected in 5-minute epochs for a test duration of 60 minutes. Total motor activity was a combination of fine motor skills (i.e. grooming, interruption of one photobeam) and ambulatory motor activity (interruption of 2 or more consecutive photobeams). Clinical Pathology: Blood samples were collected for hematology and serum chemistry from non-fasted rats, 6/sex/group at scheduled necropsies; study week 5 for males and LD 4 for females. Necropsy: Males were sacrificed following completion of the mating period (approx. wk 5). Females that delivered were sacrificed on LD4, and the numbers of former implantation sites and corpora lutea were recorded. Females that failed to deliver were sacrificed on postmating day 25 (females with evidence of mating) or post-cohabitation day 25 (females without evidence of mating). Uteri were stained with 10% ammonium sulfide for detection of early implantation loss. Females with total litter loss were sacrificed within 24 hrs of total loss. The following organs were weighed for all parental animals: adrenal glands, brain, heart, kidneys, liver, lungs, spleen, thymus, thyroids with parathyroids, testes, epididymides, prostate, ovaries with oviduct and uterus. Thirty-nine tissues and all gross lesions were collected and fixed in 10% neutral-buffered formalin, except for testes, which were fixed in Bouin's solution. Histopathology: Slides were prepared for protocol specified tissues and stained with hematoxylin-eosin, except for testes, which were stained with PAS. Microscopic evaluation was performed on all tissues from the control and 320mg/kg/day groups and on kidney, liver and thyroid glands in males and thyroid and thymus glands from females in the 20 and 80mg/kg/day groups. F1 Litter observations: Each litter was examined daily for survival. Pups were individually identified by digit tattoo. Intact offspring that died were necropsied using a fresh dissection technique including heart and major vessels. Each living pup was examined, sexed and weighed on LD1 and 4, and monitored for abnormalities in nursing behavior. Mean pup weights were presented by sex for each litter and by dose group. Litter parameter calculations included mean litter size, postnatal survival between birth and postnatal day 0 or birth and postnatal day 4 as percentage of litters, and % litters postnatal survival for all other intervals (PND0-1 and 1-4).
Results: NOAEL (NOEL)	Parental systemic NOAEL = 20mg/kg/day Reproductive NOAEL = 20mg/kg/day Neonatal toxicity NOAEL = 320mg/kg/day
LOAEL (LOEL)	Parental systemic LOAEL = 80mg/kg/day [decreased body wt and/or food consumption, organ wt changes and microscopic findings in 320mg/kg/day organs] Reproductive LOAEL = 80mg/kg/day [extended gestation, decreased number of implantations and pups born, and decreased live litter size]
Remarks	Test material: PEB Bottoms test formulations were homogeneous and contained the appropriate concentrations. Each batch of test material was stable for at least 8 days. Clinical Observations: All rats survived to scheduled necropsy. Increased

	incidence of hair loss on the ventral abdomen and/or hindlimb at daily examinations, excessive pawing of cage surfaces at time of dosing, clear or red material on body surfaces 1 hr after dosing were seen in 92% of 320mg/kg/day animals. Increased incidence of clear and/or red material around the mouth was also seen in 75% of females and 33% of males in the 80mg/kg/day group 1 hr after dosing. Clear or red material was considered to be due to potential taste aversion to the test article and not a sign of toxicity. The finding seen shortly after dosing did not persist to the next observation point. No clinical findings were observed in 20mg/kg/day rats. Body weights and Food Consumption: Mean body weight, weight gain and/or food consumption in the 80 and 320mg/kg/day group males were reduced generally throughout the study. Mean body weights in males were 13% and 8% lower and weight gain was 42% and 26% less than controls by the end of the exposure period in the 320 and 80mg/kg/day groups, respectively. Changes in food consumption varied weekly but were only statistically significantly decreased as g/animal/day during the second week of exposure in the 320mg/kg/day group males. Female body weights were not affected prior to gestation; thereafter the 320mg/kg/day pregnant animals had a 10% lower mean body weight at GD20 and 21% less weight gain over GD0-20. During the four days of lactation, mean body weight gain were reduced by 17% compared to controls and the LD 4 weight was 8% less than controls in 320mg/kg/day females. No effects were seen in groups 80 or 20mg/kg/day females. Mean food consumption in all groups of females during gestation and lactation were comparable to controls. Neurobehavioral Parameters: No significant PEB Bottoms related effects on FOB parameters or locomotor activity were observed in males during study wk 5 or females on LD 4. A statistically significant ($p<0.05$) decrease in rotarod performance in 320mg/kg/day females [59.8 ± 51.22 sec.] compared to controls [111.1 ± 21.8 sec.] was attributed to biological variation and small sample size. Only 2/6 320mg/kg/day females [remained on rotarod for <30 sec] were affected and control performance was exceptionally high [5/6 female rats remained on the rod for the entire 120 second testing period]. Historical control data for rotarod performance at the testing laboratory is approximately 86.5 ± 49.07sec for males and 76.1± 42.37 sec. for females. Clinical Pathology: Statistically significant decreases in mean absolute and/or % eosinophils were observed in 80mg/kg/day males [78% and 56% of control values, respectively] and 320mg/kg/day animals of both sexes [approximately 50% of both parameters]. No other hematology finding were observed; serum chemistry parameters were unaffected by treatment at all dose levels. Necropsy and Pathology: Increases of 10% in mean absolute and 20-25% relative kidney weights in 80 and 320mg/kg/day males correlated with mineralization, multifocal deposits and irregular basophilic material in kidneys of 320mg/kg/day males examined microscopically. Increases of 20% in mean absolute and 27-37% relative liver weights in 320mg/kg/day males and females correlated with hepatocellular hypertrophy observed microscopically. Follicular cell hypertrophy was observed in thyroid gland of 320mg/kg males and females, which correlated with increased thyroid gland weighs of 10-15% compared to controls in this group. Atrophy of the thymus was observed in 3 females in the 320mg/kg/day group correlating with decreased thymus weight of approximately 23% in these animals but no atrophy was seen in male thymus although thymus weight was decreased by 17% in these rats. No PEB Bottoms related

	microscopic findings were seen in organs examined from 20 or 80 mg/kg/day group animals. Reproduction Parameters: No effects were observed on male and female mating, fertility and copulation/conception indices. Mean number of days to mating were unaffected by PEB Bottoms treatment. Mean gestation length in the 320mg/kg/day female (22.6 days) was statistically significantly increased ($p<0.01$) compared to controls (21.6 days). One female in this group delivered a single pup on gestation day 24 that was found dead on the day of delivery. At necropsy, the mean number of implantation sites was decreased in 80 and 320mg/kg/day groups, 14.6 and 14.4 /dam, respectively compared to controls (16.0/dam). However, since the decrease in the 80mg/kg/day group was due to one female with only 8 implantation sites, the effect was attributed to biological variation in this group. The mean number of unaccounted for sites was increased in the 320mg/kg/day group (2.2/dam) compared to control (1.0/dam). The mean numbers of pups born and live litter sizes on postnatal day 0 were reduced in the 80 and 320mg/kg/day groups. Values for the 80mg/kg/day group were 13.3 mean pups born and 13.3 mean live litter size [10 litters], and for the 320mg/kg/day group were 12.2 mean pups born and 11.9 mean live litter size [11 litters] compared to control values of 15.0 mean pups born and 15.0 mean live litter size [11 litters]. None of these findings was statistically significant. F1 Litter: No PEB Bottoms related effect on the percentage of males at birth or postnatal survival was noted at any dose level. The general physical condition and mean pup body weights were unaffected by PEB Bottoms treatment of parental animals at any dose level. There were no PEB Bottoms-related findings on pups found dead or at scheduled necropsy on postnatal day 4.
Conclusions: (Laboratory contractor)	PEB Bottoms induced both parental systemic toxicity and some evidence of reproductive toxicity in treated rats. Systemic toxicity was expressed as decrements in body weight and weight gain, some decreased food consumption and changes in organ weights at 80 and 320mg/kg/day groups with correlative microscopic findings in 320mg/kg/day animals. Reproductive changes included extended mean gestation length in 320mg/kg/day females and observed decreases in implantation sites, numbers of pups born and live litter size in 80 and 320mg/kg/day groups and increased unaccounted for sites at 320mg/kg/day. Although the changes in implantation sites, unaccounted for sites, pups born and live litter size were not statistically significant, these dose related occurrences were considered biologically significant for this screening test.
Reliability:	**1.** Reliable without restriction
Reference:	A Combined 28-day Repeated Dose Oral Toxicity Study with the Reproductive/Developmental Toxicity Screening Test of Polyethylbenzene Bottoms Stream (PEB) in Rats. 2005. Wilson, D.T. and Nemec, M. (Study No. WIL-186034). WIL Research Laboratories, LLC, Ashland OH. Sponsor: American Chemistry Council, Arlington, VA
Other (source) Last changed	 1/31/06

4.1.5 Genetic Toxicity –In Vitro: Gene mutation

Test Substance:	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	OECD Guideline 471 (1998)
Type (test type):	Bacterial Reverse Mutation Assay
System of testing	*Salmonella typhimurium, E. coli*: plate incorporation ±S9
GLP:	Yes
Year (study performed):	2005
Species/Strain	*Sal. typhimurium* strains TA 1535, 1537, 100, 98 and *E. coli* WP2uvrA
Metabolic activation	Yes
Species and Cell type	Sprague Dawley rat liver homogenate (S9)
Quantity	10% homogenate in S9 mix
Induced or not induced	Livers from rats induced with Aroclor 1254 by single 500mg/kg IP injection, 5 days prior to sacrifice
Concentrations tested	0, 1.5 to 5000µg/plate in several assays
Statistical Methods:	Not applicable. Criteria for positive response are a dose-related increase in mean revertants per plate in at least one tester strain over a minimum of 2 increasing concentrations. Results were positive for TA1535 and TA1537 if the peak of the dose response was ≥ 3-fold the mean vehicle control value; for TA100, TA98 and *E. coli* WP2 uvrA if the peak of the dose response was ≥ 2-fold the mean vehicle control value.
Test Conditions	The PEB sample was a blend of equal volumes of six PEB samples from different suppliers. PEB diluted in ethanol (EtOH) was tested in 4 strains of *Salmonella* and *E. coli* WP2 uvrA with and without S9 metabolic activation in an initial toxicity/mutagenicity test (2 plates/dose) and 3 confirmatory mutagenicity assays (3 plates/dose). Doses of PEB solubilized in EtOH formed a clear, soluble solution at 500mg/ml, the highest concentration prepared. In the initial toxicity/mutagenicity trial (B1) - all *Salmonella* strains and *E. coli*, ±S9, doses were 0, 1.5, 5.0, 15, 50, 150, 500, 1500, 5000µg/plate. In the first mutagenicity trial (B2) – all *Salmonella* strains and *E. coli* ±S9, doses were 0, 15, 50, 150, 500, 1500, 5000µg/plate. The next trial (B3) was aborted due to unacceptable vehicle controls. Confirmatory trial B4 tested TA 98±S9 at doses of 0, 15, 50, 150, 500, 1500, 5000ug/plate and TA100 +S9 at 0, 50, 150, 500, 1500, 2000, 3000, 5000ug/plate. To verify mutagenic activity seen with TA100+S9, trial B5 was performed in TA100 ±S9 at doses of 0, 50, 150, 500, 1500, 2000, 3000, 5000µg/plate. Two other repeat assays using TA100 and PEB demonstrated severe toxicity over a range of doses without evidence of mutagenicity and were not considered definitive for this assay. In all assays 50µl PEB in ethanol at appropriate concentrations or vehicle was introduced into molten minimal top agar (45± 2^0C), along with 100µl of bacterial tester strain (10^9 cells/ml), 0.5ml of S9 mix or sham mix, blended by vortexing, and poured onto the surface of a 25ml

	solid minimal bottom agar plate. When top agar had set, plates were inverted and incubated for 48-72hrs at 37±2^{0}C. At the end of incubation, plates were evaluated for toxicity to background lawn and revertant colonies were counted. Replica plating was performed as appropriate to verify presence of mutant colonies from the original test plate. Positive control compounds for assays were 2-amino anthracene for +S9 plates for all *Salmonella* strains and *E. coli*; for –S9 plates, TA98, 2-nitrofluorene; TA100 and TA1535, sodium azide; TA1537, 9-aminoacridine; *E. coli* WP2 uvrA, methyl methane sulfonate.
Results: Genotoxic effects	In the initial toxicity/mutagenicity trial (B1), toxicity [reduction] to background lawn was visible at 5000µg/plate in all *Salmonella* strains and observed as a slight reduction in lawn at ≥ 500 or ≥ 1500µg/plate depending on strain and precipitate was observed beginning at 1500µg/plate ±S9 in all strains. In *E. coli*, no lawn reduction was seen and precipitate was observed beginning at 1500 µg/plate ±S. TA100 demonstrated a positive mutagenic response of 2.3 fold maximum increase above controls with S9 and 2.1 fold increase above controls without S9 at 5000ug/plate. No other *Salmonella* strain or *E. coli* showed revertant numbers in excess of negative control values. In mutagenicity trial B2 using all strains ±S9 no positive response was observed in any strain. Toxicity was observed beginning at 500 or 1500µg/plate depending on the strain and precipitate was seen beginning at 500 or 1500µg/plate. Slight reduction in background lawn was observed at 5000µg/plate in *E. coli* ±S9. Trial B4 was performed with TA100+ S9 due to severe toxicity at 1500 and 5000µg/plate not seen in TA100-S9, and with TA98±S9 due to numerous microcolonies that obscured accurate counting in the previous trial. In this test, TA98 did not demonstrate any increases in mutant colonies above controls at any dose level ±S9. TA100+S9 showed a positive response with 2.1 to 2.4-fold increases above control values at 1500, 2000, 3000 and 5000µg/plate. To confirm the mutagenic activity in TA100, trial B5 was performed with TA100 ±S9. No increase in revertant colonies of 2-fold or greater was seen with TA100-S9. The weak positive response seen with TA100 – S9 in trial B1 was not reproduced in trials B2 or B5. TA100+S9 again demonstrated a positive mutagenic response of 2.2 to 2.9-fold increase over negative control values at 1500, 2000, 3000 and 5000µg/plate. All positive control compounds demonstrated appropriate mutagenic activity in all assays.
Conclusion: (Laboratory contractor)	PEB induced a positive repeatable mutagenic response in *Salmonella typhimurium* TA100 with metabolic activation. The increase did not exceed 2.9 fold of negative controls in any trial. No other *Salmonella* strain or *E. coli* demonstrated mutagenic activity. PEB is a bacterial gene mutagen in this test system.
Reliability	**1.** Reliable without restriction
Reference	Bacterial Reverse Mutation Assay – Polyethylbenzene Bottom Stream (PEB), CAS No. 68987-42-8. 2005. San, R.H.C. and Klug, M.L. [AB00CN.503.BTL; Sponsor Project No. WIL-186036] BioReliance, Rockville, MD. Sponsor: American Chemistry Council, Arlington, VA.
Other (source) Last changed	1/31/06

4.1.5 Genetic Toxicity –In Vitro: Chromosome Aberrations

Test Substance:	Polyethylbenzene Bottoms Stream (PEB) is 100% of the complex mixture CAS RN. 68987-42-8. PEB is a coproduct of ethylbenzene manufacture and a Class II complex mixture consisting of various isomers of alkylbenzene and diphenyl hydrocarbons.
Method/Guideline:	OECD Guideline 473 (1998)
Type (test type):	Mammalian cell Chromosome Aberration test
System of testing	Rodent cells in culture
GLP:	Yes
Year (study performed):	2005
Species/Strain	Chinese Hamster Ovary (CHO) cells
Metabolic activation	Yes
Species and Cell type	Sprague Dawley rat liver homogenate (S9)
Quantity	20µl S9/ml McCoy's 5A culture medium
Induced or not induced	Livers from rats induced with Aroclor 1254 by single 500mg/kg IP injection, 5 days prior to sacrifice
Concentrations tested	Preliminary toxicity: 0, 15 to 5000µg/ml; Chromosome assay: 0, 3.13 to 150µg/ml. Analyzed doses: 0. 6.25, 12.5 and 25.0µg/ml
Statistical Methods:	Percent of aberrant cells analyzed by Fisher's exact test (p=0.05), then Cochran-Armitage to measure dose responsiveness.
Test Conditions	The PEB sample was a blend of equal volumes of six PEB samples from different suppliers. PEB diluted in ethanol (EtOH) was administered to CHO cells (5×10^5 cells/ $25cm^2$ flask) ±S9 to determine possible induction of chromosome damage in cultured mammalian cells. Cells were seeded in flasks containing McCoy's 5A medium supplemented with 10% fetal bovine serum, antibiotics and L-glutamine. For testing, cells were refed with S9 reaction mixture [S9 homogenate + co-factors] at 1ml volume in 4ml serum-free medium or with 5ml complete medium for non-activated assays, as appropriate. Test article or solvent was then added at 50µl. Osmolality in treatment medium with solvent, highest PEB concentration, lowest PEB concentrations causing precipitate or highest soluble PEB concentration was measured. The pH of the highest concentration of dosing solution in medium was also determined with pH test tape. Preliminary Toxicity assay: CHO cells were exposed to EtOH (solvent-negative control) or 9 concentrations of PEB ±S9 for 4 hrs, or without S9 for 20hrs continuously. Cells were incubated at 37 ± 1^0C in a humidified atmosphere of 5±1% CO_2 in air. After the 4 hr exposure, cells were washed, resuspended in complete medium and incubated for a total of 20 hrs from initiation of treatment. After 20 hrs, cells were harvested, trypsinized and counted using a Coulter Counter. Cell viability was determined by trypan blue dye exclusion. Chromosome Aberration test: Duplicate cultures of CHO cells were exposed to PEB ±S9. In the initial and repeat non-activated assays, cells were exposed for 4 hr or 20 hr continuously at 37 ± 1^0C and all cultures were incubated for 20hr total.

	Two hours prior to harvest, cells were treated with Colcemid® at a final concentrations of 0.1µg/ml medium. In the initial and repeat S9-activated assays, cells were exposed to PEB for 4 hrs, treatment medium was removed, cells were washed, refed and incubated for a total of 20hrs. Positive control compounds were mitomycin C [0.1 and 0.2 µg/ml] for non-activated cultures and cyclophosphamide [10 and 20µg/ml] for activated cultures. A concurrent toxicity test ±S9 was performed using an aliquot of cell suspension from each culture flask collected at cell harvest, to determine cell growth inhibition. At harvest, cells were collected by trypsinization and centrifugation at 800rpm for 5 min. Cell pellet was resuspended in 2-4ml 0.075M KCl and allowed to stand at room temperature for 4-8 min. Cells were recentrifuged, supernatant aspirated and cells fixed with 2 washes of 2ml Carnoy's fixative (methanol:glacial acetic acid, 3:1, v/v) Cells were stored overnight in fixative at approx. 2-8^{0}C. In the morning, cells were centrifuged at 800rpm for 5 min and medium changed twice; after decanting the second fixative supernatant, cells were resuspended to opalescence in fresh fixative and a small aliquot was dropped onto the center of a clean glass slide and allowed to air dry. Slides were stained with 5% Giemsa, air dried and permanently mounted. Slides were identified by study number, date and treatment condition. Analysis: The highest dose level selected for analysis of chromosome aberrations was the dose that induced at least 50% toxicity as measured by mitotic inhibition relative to solvent controls with a sufficient number of scorable metaphase cells. Two additional lower dose levels were also evaluated. Slides were coded using random numbers by an individual not involved with the study and evaluated "blind" by the cytogeneticist. A minimum of 200 metaphase spreads [100 per duplicate flask] were scored for chromatid and chromosome-type aberrations. Pulverized chromosomes and severely damaged cells (≥10 aberrations) were recorded. Numerical aberrations (polyploidy and endoreduplication) were also recorded. Chromatid gaps were recorded but not included in the analysis.
Results: Genotoxic effects	Preliminary Toxicity: Dose levels for the chromosome aberration assay were selected following a preliminary toxicity test based on reduction in cell growth relative to solvent control. Visible precipitate was observed at dose levels ≥ 150µg/ml, dose levels ≤ 50µg/ml were soluble in treatment medium at the beginning and conclusion of the treatment period. Osmolalities for treatment groups were within 2-3% of solvent control, pH = 7.0 in all treated flasks. Substantial toxicity occurred at ≥ 150µg/ml in non-activated 4 and 20 hr exposure groups and at levels ≥ 50µg/ml in S9 activated 4 hr exposure groups. Chromosome aberration assay: Dose levels selected for all treatment regimens were 0, 3.13, 6.25, 12.5, 25, 50, 75, 100, 125 and 150µg/ml. Visible precipitate was observed at dose levels ≥ 100µg/ml; dose levels ≤ 75µg/ml were soluble in treatment medium and the beginning and conclusion of treatment. Osmolality and pH of treated cultures were comparable to controls. 4hr exposure –S9: Dose levels evaluated were 6.25, 12.5, and 25µg/ml. Mitotic Index at 25µg/ml was reduced 52% relative to solvent controls. The percentage of cells with numerical or structural anomalies was not significantly increased above solvent control values at any dose level. 4hr exposure +S9: Dose levels evaluated were 3.13, 6.25, and 12.5µg/ml. Mitotic Index at 12.5µg/ml was reduced 53% relative to solvent controls. The percentage of cells with numerical or structural anomalies was not significantly increased above solvent control values at any dose level.

	20hr exposure –S9: Dose levels evaluated were 6.25, 12.5, and 25µg/ml. Mitotic Index at 25µg/ml was reduced 54% relative to solvent controls. The percentage of cells with structural anomalies was not significantly increased above solvent control values at any dose level. The percentage of cells with numerical aberrations (polyploidy and/or endoreduplication) was statistically significantly increased at dose levels of 12.5 and 25µg/ml [$p \leq 0.05$, Fischer's Exact test] but no dose response was seen in the Cochran-Armitage test. Since the percentage of cells with numerical aberrations at dose levels 12.5 (7.5%) and 25ug/ml (7.0%) were within the historical control range of 0.0 to 7.5% for this laboratory and there was no increasing dose response, this effect was not considered biologically significant. Confirmatory test for absence of effect with metabolic activation: A repeat test was performed with a 4 hr exposure +S9. Dose levels evaluated were 6.25, 12.5, and 25µg/ml. Mitotic Index at 25µg/ml was reduced 53% relative to solvent controls. The percentage of cells with numerical or structural anomalies were not significantly increased above solvent control values at any dose level. Positive control compounds in all assays demonstrated appropriate clastogenic activity.
Conclusion: (Laboratory contractor)	PEB is not clastogenic to mammalian cells in culture. No biologically significant increases in structural or numerical aberrations were observed in chromosomes at any dose levels in any exposure regimen.
Reliability	**1.** Reliable without restriction
Reference	*In Vitro* Chromosome Aberration Test – Polyethylbenzene Bottom Stream (PEB), CAS No. 68987-42-8. 2005. Gudi, R., and Rao, M. [AB00CN.331.BTL; Sponsor Project No. WIL-186037] BioReliance, Rockville, MD. Sponsor: American Chemistry Council, Arlington, VA.
Other (source) Last changed	1/31/06